The Metropolis algorithm for on-shell four-momentum phase space

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Abstract

We present several implementations of the Metropolis method, an adaptive Monte Carlo algorithm, which allow for the calculation of multi-dimensional integrals over arbitrary on-shell four-momentum phase space. The Metropolis technique reveals itself very suitable for the treatment of high energy processes in particle physics, particularly when the number of final state objects and of kinematic constraints on the latter gets larger. We compare the performances of the Metropolis algorithm with those of other programs widely used in numerical simulations.

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1 Introduction

Over the past few years, high energy particle physics has experienced a tremendous advance in the number of methods developed to calculate exactly scattering and decay amplitudes of elementary processes. Several techniques exist nowadays to evaluate matrix elements (MEs) for multi-particle events, both analytical and numerical, no matter the actual number of particles involved.

However, in phenomenological studies, the evaluation of the MEs, in terms of the external particle momenta, is only a part of the whole story. In fact, in order to perform realistic analyses, given the finite resolution of particle detectors, a multi-dimensional integration over the whole or some region of the phase space available to the final state particles has to be performed. Indeed, in most cases, an analytical evaluation of the integrals becomes extremely complicated, if not impossible, either because of the complexity of the integrand and the large number of dimensions involved or because of the presence of cuts in the integration region.

In such cases, one has to necessarily rely on numerical methods. Moreover, as the dimension of the integral increases, the number of evaluations of the integrand function needed in any generalised one-dimensional numerical approach inevitably grows exponentially. Therefore, the recourse to Monte Carlo (MC) methods becomes mandatory: it is well known that the rate of convergence of MC algorithms is independent of the dimensionality of the integral.

Naive MC algorithms are typically based on estimating the average value of the integrand function by sampling the latter at discrete points generated according to a uniform statistical (i.e., random) distribution. However, this approach turns out to be unsatisfactory if the integrand function strongly fluctuates over the integration volume, as it is the case in many high energy particle processes. Thus, a strategy that reduces the variance of the integrand ought to be incorporated, in order to improve upon the tendency to converge to the correct value (see Ref. for details).

Two approaches have become popular to this end, known as stratified and importance sampling. Whereas in the latter case the algorithm concentrates where the integrand is largest in magnitude, in the former the function is primarily sampled where the contribution to the error is largest. Both techniques suffer however from a shortcoming: namely, the need to know beforehand the behaviour of the integrand over the all integration volume, in order to optimise the implementation. Unfortunately, it is exactly this knowledge that is often missing in particle physics phenomenology.

1Besides, in hadron-hadron and lepton-hadron collisions, the integration over the Parton Distribution Functions (PDFs) cannot be performed analytically, as these are accounted for by programs implementing numerical fits to various data sets.
A successful way of improving in this respect is represented by adaptive procedures. These normally involve a division of the original integration region into a predetermined number of ‘bins’ (word that we adopt here to signify any partition of the integration volume), with a certain number of points in each of these, the latter being at times redefined so to perform importance sampling automatically. A very much used example of such a technique is the program VEGAS\cite{3}. As a matter of fact, VEGAS also makes use of some stratified sampling, in order to improve the convergence in low dimensions. Because of its efficiency and accuracy, this algorithm has eventually come to set the standard in many particle physics calculations\footnote{For parallel versions of VEGAS, see Ref.\cite{4}.}

The appearance of large fluctuations in the integrand is often associated to the presence of ‘singularities’ in the MEs. In this respect, one can broadly distinguish between integrable singularities (e.g., resonances) inside the phase space and non-integrable ones (e.g., infrared emissions) at its borders. Taken separately, they may both be considered as ‘factorisable’. In the sense that, provided a suitable choice (or mapping) of the integration variables is adopted, then the integrand can be transformed into a smoother function everywhere over the space space, with the MC points being generated according to a (suitable) non-uniform probability density. In many examples in high energy physics, however, the two kind of poles can occur at the same time and, possibly, there can be more than one of each type: particularly, as the number of final state particles, their nature and their production channels proliferate. Under these circumstances, the singular structure of the integrand becomes ‘non-factorisable’, in the sense that there generally exists no change of variables that allows even the adaptive algorithm to sample simultaneously all the singularities of the integrand in an efficient manner. A multi-channel approach can prove useful in such cases\cite{5}. Here, the actual mapping used to generate a single event is chosen randomly, using a predetermined set of probabilities (or weights). A combination of the VEGAS algorithm with the adaptive multi-channel sampling of Ref.\cite{4} has recently been proposed\cite{6}.

Another example of adaptive MC algorithm is the Metropolis technique\cite{7}. Widely used in statistical physics (see Ref.\cite{8} for a review), it has nonetheless seen very little applications to particle physics. These have been mainly confined to the case of Lattice Gauge Theories (LGTs)\cite{9}. It is our intention here to demonstrate its potential in the context of a Quantum Field Theory (QFT) of the continuum: in evaluating total and differential cross sections in multi-particle scattering processes at high energies. In particular, we will show how a Metropolis algorithm easily lends itself to several manipulations, that make it a versatile instrument in performing such calculations, thus overcoming most of the problems that we have described, often matching in speed, efficiency and accuracy VEGAS itself and outclassing many others of the most commonly used algorithms.
The plan of the paper is as follows. In Sect. 2 we describe the fundamentals of the Metropolis technique and propose several integration methods. Sect. 3 presents a few numerical examples and comparisons with other algorithms in the context of some benchmark processes in high energy particle physics. In Sect. 4 we summarise our results. Finally, we will defer to the Appendix the analytical proof of a condition required to the algorithm for its convergence in four-momentum phase space.

2 The Metropolis algorithm for a QFT

The Metropolis method [7] is a somewhat adaptive MC integration algorithm which is widely used in numerical statistical mechanics and LGTs. We will here demonstrate how it can be modified to evaluate cross sections and other observables from perturbative ME calculations of scattering and decay processes in a QFT. The integration is performed over the four-momentum phase space of the final state particles. The phase space can be of arbitrary form, with the only requirement that the particles are on their mass-shell, i.e., \( p_i^2 = m_i^2 = \text{constant} \), where \( p_i \) and \( m_i \) represent the four-momentum and mass of the \( i \)-th particle. This restriction is enforced by construction, in order to give a correct description of the phase space associated to the final state particles. However, intermediate particles, that can appear in a process, are allowed to be off-shell.

2.1 Description of the algorithm

In general, the problem is defined by a phase space and a weight-function \( w(x) \) for every point \( x \) in phase space. A random walk in the phase space is performed by starting at an arbitrary initial point \( x_0 \), and generating new points \( x_i \) by using the weight \( w \). In the Metropolis algorithm, the sequence \( \{x_i\} \) is generated in a way which ensures that the points will reach the correct distribution when the number of steps (hereafter, \( N \)) is large. In a QFT, the phase space is given by the on-shell four-momenta of the outgoing (and possibly incoming) particles, the weight-function coincides with the ME, and the cross section will correspond to the partition function (defined below) of the problem.

In [7] it is shown that in order to reach the correct probability distribution, \( P(x) \propto w(x)dx \), for the sequence, one has to fulfill two conditions in the stepping procedure \( x_i \rightarrow x_{i+1} \).

\(^3\)In statistical mechanics, \( w \) is normally given by an energy-function, a temperature and the Boltzmann distribution.
(a) All points in phase space must be reachable with a finite number of steps.

(b) The condition of ‘detailed balance’ must be fulfilled:

\[ P(x_i)P(x_i \rightarrow x_{i+1}) = P(x_{i+1})P(x_{i+1} \rightarrow x_i). \]

The normal procedure to satisfy detailed balance (b) is to randomly choose a point \( \tilde{x}_{i+1} \) with even distribution inside a region \( \Omega_i \). This new point is then accepted with probability

\[ P = \min(1, \frac{w(\tilde{x}_{i+1})}{w(x_i)}). \]

If it is not accepted, the previous point will be put in the sequence once more: i.e., \( x_{i+1} = x_i \). Condition (a) is then satisfied if the overlap of \( \{ \Omega_i \} \) can cover the whole of the phase space. Choosing the \( \Omega_i \)'s to actually be smaller than the phase space will make the Metropolis algorithm adaptive since, at each step, the suggested point \( \tilde{x}_{i+1} \) is likely to be in the region of large weights.

For any observable, \( \mathcal{O}(x) \), the mean can then be calculated as follows:

\[ <\mathcal{O}>_w \equiv \frac{\int \mathcal{O}(x)w(x)dx}{\int w(x)dx} = \lim_{N \to \infty} \frac{\sum_1^N \mathcal{O}(x_i)}{N}. \] (1)

The partition function, \( Z \), can be calculated by evaluating the average of \( 1/w \) and using the relation:

\[ Z \equiv \int w(x)dx = \frac{\int dx}{<1/w>_w}. \] (2)

However, a straightforward use of the Metropolis algorithm will in this case be inefficient since \( 1/w \) has large contributions when \( w \) is small. The regions of small \( w \) are not visited so often, and one would have large statistical fluctuations. For a \( w \) that has large variations, it is then better to weight the random walk with \( w^{1/2} \) instead, and to evaluate \( Z \) by:

\[ Z \equiv \int w(x)dx = \frac{\int dx}{<w^{1/2}>_w}. \] (3)

In this way, the magnitude of the variations in the weight-function are effectively halved. The total volume of phase space, \( \int dx \), has to be estimated separately.

In a QFT one is often interested in evaluating the total cross section other than observables of the four-momenta. For example, for processes with two particles in the initial and \( n \) in the final state (scattering reactions), the cross section can be written as

\[ \sigma = \frac{(2\pi)^4}{2p_{tot}^2} \int |\mathcal{M}|^2(p_a, p_b, \{p_i\}) \prod_{i=1}^n \left[ \frac{d^4p_i}{(2\pi)^3} \delta^+(p_i^2 - m_i^2) \right] \delta(p_{tot} - \sum p_i), \] (4)

where \( p_{tot} \) is the total four-momentum, \( p_a \) and \( p_b \) are the incoming momenta, \( \{p_i\} \) are the \( n \) final state momenta, with \( m_i \) their respective masses, and \( |\mathcal{M}|^2 \) the ME
associated to the reaction considered. By choosing the weight-function and the phase space to be

\[ w = \frac{(2\pi)^{4-3n}}{2p_{tot}^2} |\mathcal{M}|^2(p_a, p_b, \{p_i\}), \]

\[ dx = \prod_{i=1}^{n} \left[ d^4p_i \delta^+(p_i^2 - m_i^2) \right] \delta(p_{tot} - \sum p_i), \]

respectively, we can use the Metropolis algorithm to perform the integration.

In order to do so, one has to guarantee that the stepping procedure in the Lorentz-invariant phase space (6) can be done in a way that satisfies the two conditions (a) and (b) above. We now describe how this can be achieved: first comes an illustration (points (i) to (iv)) of how the suggested point in phase space, \( \tilde{x}_{i+1} \), can be generated; afterwards, we show that this procedure complies with (a) and (b).

The proposed point in phase space, \( \tilde{x}_{i+1} \), can be generated in the following way.

(i) Choose two of the final state particles randomly.

(ii) Boost them into their centre-of-mass (CM) frame.

(iii) In that frame, rotate them randomly with an even distribution in \( 4\pi \).

(iv) Boost them back into the original frame.

In order to demonstrate that this procedure will satisfy conditions (a) and (b), we will make use of the Lorentz-invariance of \( dx \) in eq. (6). To make sure that (b) is fulfilled, we have to show that the suggested point is generated with an even distribution inside the region \( \Omega \), which is reachable in one step. But it is clear that this is true in the CM frame of the two particles chosen in (i). Therefore, and because of Lorentz-invariance, it is true in any frame.

To demonstrate that also condition (a) is fulfilled, we have to show that from any point in phase space, \( \{p_i\} \), one can reach any other point, \( \{p'_i\} \), by a finite number of steps. This can actually be achieved in, at most, \( n - 1 \) steps. Let \( \Delta p_i \) be the shift of the \( i \)-th four-momentum, \( p'_i = p_i + \Delta p_i \). Choose an arbitrary particle, say \( p_n \). For each of the \( n - 1 \) other momenta, \( \Delta p_i \) can be transferred to \( p_n \) in one step. This is clear since \( p_i + p_n \) is conserved. In the CM frame of \( p_i \) and \( p_n \), the whole surface of conserved \( p_i + p_n \) and the other momenta fixed can be reached in one step. So is in any frame: any \( \Delta p_i \) which conserves \( p_i + p_n \) can be transferred in one step. By doing this for all the \( n - 1 \) other particles, we have reached the point \( \{p'_i\} \).

In some cases, one might want to introduce cuts in the integration volume\(^4\). That is, instead of integrating over the whole of phase space, \( PS \), one might want to

\(^4\)Alternatively, the ME might be identically zero inside a finite region of it.
integrate inside a reduced region, $P_{S_{\text{red}}}$. In that case, one has to make sure that condition (a) is fulfilled also over $P_{S_{\text{red}}}$. In the Appendix we show that this is the case if $P_{S_{\text{red}}}$ is a connected region. If this is not true, then $P_{S_{\text{red}}}$ has to be separated into parts, $P_{S_{\text{red}},i}$, each of which is connected, and the integration be done for each of these separately.

Finally, in some cases, it can be desirable to integrate a ME (or just a term of it, in which case we use the notation $T$) which is negative over some parts of the phase space. If so, $T$ can not directly be used as the weight-function $w$. Instead, one can use its absolute value, and keep track of how often $T$ is negative. With $w = |T|$, the partition function is in this case given by:

$$Z = \frac{\langle \text{sign}(T) \rangle_{w^{1/2}}}{\langle w^{-1/2} \rangle_{w^{1/2}}} \int dx.$$  \hspace{1cm} (7)

In summary, the average of an observable $O$, given by a function $O(\{p_i\})$, can be calculated as follows.

- Choose a suitable starting point $\{p_{i0}\}$.
- Generate a new point $\{\tilde{p}_{i1}\}$ as described above.
- Accept this point with the probability
  $$P(\{p_{i1}\} = \{\tilde{p}_{i1}\}) = \min \left( 1, \frac{w(\{\tilde{p}_{i1}\})}{w(\{p_{i0}\})} \right),$$
  with $w$ given by the ME (eq. (5)).
- If not accepted, use the previous point: $\{p_{i1}\} = \{p_{i0}\}$.
- Store the value of $O$: $O_{\text{sum}} = O_{\text{sum}} + O(\{p_{i1}\})$.
- Repeat the four last steps until the desired level of convergence is reached ($N$ steps).
- Finally, take the average: $<O> \approx \frac{O_{\text{sum}}}{N}$.

### 2.2 Time consumption and error estimates

In most of the (sub)processes that we have integrated with the Metropolis algorithm, the, by far, most time-consuming tasks have been the calls to the ME function. Our strategy to reduce the CPU-time has then been to, as far as possible, reduce the error for a fixed number of calls to this function.
The algorithm requires many boosts and rotations of four-vectors. For 1 million steps through phase space, e.g., this takes around 30 seconds on a 350 MHz Pentium-II processor, on a LINUX platform. Calling the ME the same number of times on the same machine is often a matter of hours. Thus, the stepping procedure has not been optimised. Instead, we have tried different ways of refining the interface between the algorithm itself and its use of the ME.

A complication in evaluating the statistical error in a Metropolis-based integration is that the generated points in phase space are correlated. The correlation length effectively reduces the number of statistically independent data points. We have handled this flaw by collecting the data into a number of ‘blocks’. The average in each block is then taken and used as a new, statistically independent data point. The size of the blocks must be made larger than the correlation length, while the number of blocks must be large enough, so that the variance evaluated from the averages can be trusted. The normal procedure to check that the correlation length has been reached is to divide each blocks into smaller parts, and check that single block-parts inside one block are not more correlated than the block-parts from different blocks, see Ref. [10].

2.3 Some methods of refinement

In this Subsection, we will describe some methods of refinement which are devoted to reduce the error in the integration for a certain number of calls to the ME. These methods will in general increase the CPU-time of the algorithm significantly, but, as mentioned above, the overall CPU-consumption will increase marginally, while improving the efficiency of the algorithm in various respects.

2.3.1 The parallel integration method

In realistic problems, the ME can present large variations, often due to resonances arising from intermediate particles. In simple terms, large variations make it hard to move around in phase space. The correlation length in the Metropolis steps will be large and many calls to the ME will be required in order to get independent data points. We will here describe a method, the ‘parallel integration method’, which enables one to move large distances in phase space, without using the exact (time consuming) ME function.

First, one can introduce an approximate ME, $|\tilde{M}|^2(x)$. This should be a simple function which is quick to call, and which is a good approximation in the regions where $|M|^2(x)$ has large contributions. It could, e.g., be a product of just the

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5Hereafter, denoted by the short-hand notation $|M|^2(x) \equiv |M|^2(p_\alpha, p_\beta, \{p_i\})$, where $x$ represents the phase space point $\{p_i\}$ of eq. ($\tilde{M}$).
resonant propagators in $|\mathcal{M}|^2(x)$. Then the configuration space is enlarged with an extra, discrete parameter, $s$, which can assume the values 0 or 1. A weight-function $w$ is constructed in the enlarged configuration space, such that it returns $|\mathcal{M}|^2(x)$ if $s = 1$ and $|\tilde{\mathcal{M}}|^2(x)$ if $s = 0$. Finally, the Metropolis-step is modified so that, occasionally, instead of suggesting a new set of four-momenta, a new value of $s$ is suggested. Data points are to be taken only when $s = 1$. The distributions of points in the part with $s = 1$ (of our enlarged configuration-space) will be exactly as in the original phase space but with only $|\mathcal{M}|^2(x)$ as the weight function. We know this since, in general, the Metropolis algorithm ensures that the generated points are distributed according to the weight-function, and this is of course true also for individual parts of the configuration space.

The gain of this method is that, during the steps in phase space when $s = 0$, one can reach distant points, without calling the slow, exact $|\mathcal{M}|^2(x)$. At will, one can choose to make it more probable that $s = 0$, so that $|\mathcal{M}|^2(x)$ is used as seldom as possible. For example, this can be done by introducing two integers, $N_0$ and $N_1$. If $s = i$, we attempt to switch the value of $s$ after $N_i$ steps. We can then choose, e.g., $N_0 = 100$ and $N_1 = 1$. The optimal value of $N_0/N_1$ will be given by how faster the approximate ME function actually is in comparison to the exact one.

Let us summarise the parallel integration method.

- Find a crude and quick approximation, $|\tilde{\mathcal{M}}|^2(x)$, to the original ME, $|\mathcal{M}|^2(x)$.
- Enlarge the phase space by introducing the discrete parameter $s = \{0, 1\}$.
- Construct the weight function

$$w(x, s) = \begin{cases} |\mathcal{M}|^2(x) & \text{if } s = 1, \\
|\tilde{\mathcal{M}}|^2(x) & \text{if } s = 0. \end{cases}$$

- Choose an arbitrary starting point $x_0$ in phase space and set $s = 0$\footnote{Also arbitrary, but $s = 0$ is recommended.}.
- Perform $N_0$ Metropolis steps with the weight $w(x, 0) = |\tilde{\mathcal{M}}|^2(x)$, and without collecting the value of the observable $\mathcal{O}$.
- Switch the value of $s$ with probability

$$P = \min\left(1, \frac{w(x, 1)}{w(x, 0)}\right) = \min\left(1, \frac{|\mathcal{M}|^2(x)}{|\tilde{\mathcal{M}}|^2(x)}\right).$$

- If the switch is accepted, store the value of the observable.
• The last three points are repeated in the following way until desired convergence is reached:
  
  – If $s = i$, perform $N_i$ Metropolis steps and, only if $s = 1$, store the value of $O$ after each step.
  
  – Switch the value of $s$ with the probability
    \[ P = \min\left(1, \frac{w(x, s')}{w(x, s)}\right), \]
    where $s' = 1$ if $s = 0$ and $s' = 0$ if $s = 1$.
  
  – Store the value of $O$, if the new $s = 1$.

• Take the average of the observable.

With this method, the total cross-section is calculable in a more effective way, than described before. This is the case if the cross-section of the approximate ME is already known with high accuracy. By counting the number of times, $r_i$, that $s = i$ after a switch, one gets the relative magnitudes of the cross-sections from the fraction of the $r_i$’s. If the exact cross-section is denoted by $\sigma$, and the approximate one by $\tilde{\sigma}$, one has that

\[ \sigma = \tilde{\sigma} \frac{r_1}{r_0}. \]  

(8)

2.3.2 The variable energy method

In some cases, one is interested in doing the integration with a dynamically variable total energy, $E_{\text{tot}} \neq \text{constant}$. This might be the case, e.g., if one is interested in the cross section as a function of $E_{\text{tot}}$ in a certain range, or if the two incoming particles can have varying energy, e.g., depending on some given PDF. To this end, we describe here the ‘variable energy method’, where the configuration space is extended by adding $E_{\text{tot}}$ as a dynamical parameter. Allowing for a variable energy can actually make the integration more effective, for the following reason: it is often the case that the variations of the ME are larger for larger energies. The phase space walk is thus easier at low energies. If one is interested in some observables to be calculated at large $E_{\text{tot}}$, it can be easier to reach farther in phase space by, say, taking a round tour into the lower energy regions. This idea has been explored in calculations in statistical mechanics, where often is the temperature to be used as a dynamical variable [11,12].

One proceeds as follows. Let a point in the extended configuration space be denoted by $x = (\{p_i\}, E_{\text{tot}})$, where $E_{\text{tot}}$ has been written explicitly, though it is actually computed from the four-momenta. In order to be able to dynamically take steps
to other energies, we introduce a one-to-one mapping \( \{\tilde{p}_i\} = K(\{p_i\}, \tilde{E}_{\text{tot}}) \), which gives a new point, \( (\{\tilde{p}_i\}, \tilde{E}_{\text{tot}}) \), given the previous one, \( (\{p_i\}, E_{\text{tot}}) \), and the new energy as well, \( \tilde{E}_{\text{tot}} \). We also need a phase space weight, \( \rho(\{p_i\}, E_{\text{tot}}) \rightarrow (\{\tilde{p}_i\}, \tilde{E}_{\text{tot}}) \), which is evaluated from phase space densities at the different energies (as described below). In the Metropolis path, one can alternatively attempt to change the energy or just update the configuration. A step which can change \( E_{\text{tot}} \) is then taken in the following way.

- Suggest a new energy, \( \tilde{E}_{\text{tot}} \), chosen with even distribution in a certain region.
- Find the corresponding point in phase space, \( \{\tilde{p}_i\} = K(\{p_i\}, \tilde{E}_{\text{tot}}) \).
- Accept this with probability

\[
P = \min \left( 1, \frac{|\mathcal{M}|^2(\{\tilde{p}_i\})}{|\mathcal{M}|^2(\{p_i\})} \right).
\]

How the mapping \( K \) can be defined and how the corresponding phase space weight \( \rho \) is calculated is the next step. In order to describe how this can be achieved, we have to digress briefly, by giving a general description of the Lorentz phase space, defined in eq. (6) (for an overview, see, e.g., Ref. [13]).

Let \( V_n(\{m_i\}, s) \) denote the total volume of the \( n \)-particle phase space with masses \( \{m_i\} \) at the squared invariant energy \( s \). For \( n = 2 \), we have

\[
V_2(m_1^2, m_2^2, s) = \frac{\pi}{2s} \sqrt{\lambda(m_1^2, m_2^2, s)},
\]

with \( \lambda(a, b, c) = a^2 + b^2 + c^2 - 2ab - 2bc - 2ca \). In the CM frame, the magnitude of the two outgoing momenta is given by

\[
P(m_1^2, m_2^2, s) = \frac{1}{2\sqrt{s}} \sqrt{\lambda(m_1^2, m_2^2, s)}.
\]

The volume for \( n \) particles can then be calculated recursively:

\[
V_n(\{m_i\}_n, s) = \int_{s_0}^{s_1} ds' V_2(s', m_n^2, s) V_{n-1}(\{m_i\}_{n-1}, s'),
\]

where the integration range is restricted between \( s_0 = (\sum_{i=1}^{n-1} m_i)^2 \) and \( s_1 = (\sqrt{s} - m_n)^2 \). The mapping \( K \), from the energy \( E_{\text{tot}} \) to \( \tilde{E}_{\text{tot}} = E_{\text{tot}} + \Delta E \), can be defined by changing the momentum of the \( n \)-th particle and boosting the others, so that the same CM frame is kept. In case this is actually possible, the back-to-back momentum of the \( n \)-th particle and the \( n-1 \) particle system, in the CM frame, is given by \( P(s', m_n^2, \tilde{E}_{\text{tot}}) \), with the momentum-function \( P \) as in eq. (10).
When the change in energy can be done in this way (i.e., provided $\lambda > 0$), $\rho$ is given by the ratio of the 2-particle volume for the two energies. This is the case since the value of $s'$ is preserved and the $n - 1$ particle volume in the integrand in eq. (11) is not affected. Thus, the $\rho$ expression corresponding to our mapping $K$ is given by

$$
\rho(E_{\text{tot}} \to \tilde{E}_{\text{tot}}) = \frac{V_2(s', m^2_{n_1}, \tilde{E}^2_{\text{tot}})}{V_2(s', m^2_{n_1}, E^2_{\text{tot}})} \theta(\lambda(m^2_1, m^2_2, s)),$$

where the $\theta$-function returns a zero when $\lambda < 0$ (corresponding to the case in which $s'$ is out of the integration range of eq. (11)), and 1 otherwise. We stress again that the choice of the mapping $K$ is not unique. We have illustrated here a simple method, however, it is possible that other, more sophisticated mappings can be chosen to make the whole procedure more efficient.

### 2.3.3 Variable energy and parallel integration

The two methods described above can be used simultaneously, as follows. Choose an energy interval $IE$, where the integration is to be performed, and a fixed energy, $E_p$, to be used only for the approximate ME function $|\tilde{M}|^2(x)$. Also define a smaller interval $IE_{W} \subset IE$, which will be the ‘window’ where we switch between the exact and approximate MEs. The need for such a region is induced by the fact that the cross section often varies a lot with energy. The window should be put around the region in energy where the cross section is expected to be large. It is also recommendable to have the fixed energy, $E_p$, inside this window. The algorithm then goes as for the parallel integration method except that, when the exact ME is to be used, one allows also for energy updates. We here describe how the cross section as a function of energy is evaluated, assuming that the cross section for the approximate ME, $\tilde{\sigma}(E_p)$, is known at one energy, $E_p$.

The stepping procedure is done as sketched below.

- Choose the energy ranges $IE \supset IE_{W}$, and the point $E_p \in IE_{W}$: $IE$ is the range we are interested in, $IE_{W}$ should be chosen in the region of large cross sections and $E_p$ is the point where $\tilde{\sigma}$ is known. Let, as before, $E_{\text{tot}}$ denote the latest accepted energy used for the exact ME. The starting value could, e.g., be $E_{\text{tot}} = E_p$.

- Introduce the discrete parameter, $s = \{0, 1\}$, and the two update periods, $N_0$ and $N_1$, as before.

- Start with $s = 0$ at the energy $E_p$ and perform $N_0$ ordinary Metropolis steps with the approximate ME.
• Attempt a switch of the value of $s$ by proposing an energy step $E_p \rightarrow E_{\text{tot}}$, as described in Subsect. 2.3.2, with the new weight given by the exact ME.

• Whenever $s = 1$ is accepted, an energy-varying Metropolis path is taken in the region $I E$. Whenever $N_1$ points inside the window $IE_W$ have been chosen, a new switch of $s$ is attempted to the point $E_p$ and with the approximate ME as the new weight.

In order to get an estimate for the total cross section for the exact ME, $\sigma(E)$, one needs to store the distribution of energies generated when $s = 1$. This distribution is then normalised by means of $\tilde{\sigma}(E_p)$, together with an evaluation of how often $s = 1$. That is, proceed as follows.

• Whenever $s = 1$ and an energy step inside $IE$ is taken, put the new energy into a distribution, $f(E)$.

• Evaluate the number of times, $r_i$, that the value of $s = i$, after a switch attempt.

• Do this until desired convergence of the distribution, $f(E)$, and the numbers, $r_i$, is reached.

The cross section then becomes, $\sigma(E) = N f(E)$ with the normalisation factor $N = \tilde{\sigma}(E_p) r_1 / \bar{f} r_0$, where $\bar{f}$ is the average of $f(E)$ inside the window $IE_W$.

3 Examples and performances

In this Section we report about some numerical results obtained by using the Metropolis algorithm and compare them to the outputs of other integration programs widely used in particle physics calculations. In Subsect. 3.1 we study multi-photon production in electron-positron annihilations, as an example of the ability of the various algorithms to deal with the problem of singularities associated with an increasing number of infrared emissions of different topology and over an increasingly reduced phase space. The benchmark process considered in Subsect. 3.2 is the production of $b$-quark and $W^{\pm}$-boson pairs at future lepton colliders, in order to test the performances of the algorithms in presence of massive particles and divergent/resonant invariant mass poles, the latter further occurring in a multi-channel environment where use of negative weights is made. Finally, in Subsect. 3.3, we will focus our attention to the case of some radiative top-antitop events as produced in hadron-hadron collisions, leading to eight-parton final states, the latter

\footnote{This could be the same energy as before, in case the suggested energy is not accepted.}
integrated over a reduced phase space: here, we account for the behaviour of the integrator as induced by a non-fixed partonic energy, a large number of particles in the final state and the enforcement of experimental cuts through $\theta$-functions in the integrand.

We have carried out our tests on several machines, without finding any significant dependence of the relative algorithm performances upon a particular choice among them. For reference, we list here the platforms used: $\alpha$-DECstations 3000 Model 300 and 400 and $\alpha$-Servers 1000A 5/300 and 1000 4/200 (running both VMS and OSF operating systems), UNIX Hewlett-Packard Workstations type A 9000/712 and A 9000/782 and the LINUX system already mentioned.

3.1 Multiple infrared radiation

The reference paper for this Subsection is [14]. There, it was studied the tree-level process $e^+e^- \rightarrow n \gamma$ (with massless electrons/positrons), where $\gamma$ refers to a photon with $n$ taken up to 7, and where the relevant MEs were presented analytically. In our forthcoming tests, we have made use of the expression for the latter given in eq. (17) of [14]. Notice that such a formula is exact for $n < 4$ only, whereas it is an approximation for $n \geq 4$. However, being much faster than the exact ME, eq. (16) of that paper, while retaining its main dynamic features, it is much more useful to our purposes.

The challenge here is to integrate a ME that diverges when a photon becomes either soft or collinear (with one of the initial state fermions). To render the results finite, while still allowing for the infrared behaviour at the edges of the (reduced) phase space, we impose the following cuts (same as in Ref. [14]):

$$E_\gamma > 5 \text{ GeV}, \quad \cos \theta_\gamma < 0.9,$$

(12)
on the energy and (cosine of the) polar angle of each final state photon. For comparison purposes, we also adopt the same CM energy used in [14], that is, $\sqrt{s} = 100$ GeV. However, we will increase here the number $n$ of photons produced to 9.

The algorithms used for this example, other than the Metropolis one, are VEGAS, RAMBO and the NAGLIB subroutines D01EAF and D01GCF. Of VEGAS, we have already given a description. RAMBO [15] is not exactly an integrator, though it can be used in some instances in such a fashion. Rather, it is a multi-particle phase space generator, as – given the total CM energy and the number of particles required with their masses – it produces a set of four-momenta and the phase space weight associated with that configuration. However, when the integrand function does not present sharp peaks (as it is the case here), it can be used to estimate the total cross section and its standard deviation simply as an arithmetic average and
through a standard quadrature formula, respectively. Indeed, this is the algorithm that was successfully employed in Ref. [14]. The subroutines D01EAF and D01GCF are part of the NAGLIB library [16]. They both are multi-dimensional adaptive quadrature integrators, the first over an hyper-rectangle whereas the second on a general product region. D01EAF makes use of the algorithm described in Ref. [17], whereas for D01GCF one should refer to [18]. Their usage and characteristics are well introduced in Ref. [16], so we do not dwell any longer on them. The Metropolis implementation used here is the one described in Subsect. 2.1, making use of the more effective formula in eq. (3). The reduced phase space volume (after cuts), i.e., \( \int dx \) in (3), was calculated numerically but with insignificantly small errors. Alternatively, one can assume it to be given as an exact input, if the phase space integration can be performed analytically.

In this test, we have proceeded as follows. For a start, we have fixed the number of MC points generated to carry out the integration, \( N_{MC} \), to be approximately \( 10^6 \) (including those eventually rejected because of the cuts) for all algorithms and irrespectively of the number of photons generated. One may consider this condition as a prototype of what inevitably occurs in numerical computations, when one can only dispose of a finite amount of CPU (here, corresponding to the time needed to evaluate \( 10^6 \) times the integrand function, as it would actually happen if all momentum configurations generated were accepted). Notice that we have introduced the cuts through theta functions in energy and angles, while maintaining as upper and lower limits of the integration variables those needed to cover the all of the original (massless) \( n \)-particle phase space. Under these conditions, what one would expect from an optimal algorithm is both the tendency of promptly adapting itself to an increasingly reduced integration volume – as \( n \) gets larger – (thus minimising the loss of MC points through the cuts) and the ability to efficiently dispose of those points that survive the kinematic constraints (by minimising the error of the integration). A measure of the former is the ratio between accepted and generated MC points, whereas for the latter of the percentage spread of the errors about the central values obtained. We will see that the estimates will roughly be consistent with each other for all algorithms up to \( n = 8 \), while some of the programs will fail to converge for \( n = 9 \). Then, for those programs that manifest the ability to converge to the correct value of the cross sections with good accuracy up to \( n = 9 \), we have increased \( N_{MC} \) by ten and hundred times, this way further checking the rate of convergence of the algorithms.

---

\[ \text{In fact, here the expression of the } n \text{-photon ME is considerably simple that the time spent in evaluating it has little impact on the total one employed by the all integration procedure, irrespectively of the value of } n. \]

\[ \text{For consistency, we have customised the choice of the latter to be the same invariant masses and angles for VEgas, D01EAF and D01GCF. As for RAMBO, there is no need to provide the integration variables and corresponding Jacobian factors, as this is done automatically by the program: see Ref. [15] for specific details.} \]
when, ideally, an infinite CPU (i.e., number of MC points) is made available. For sake of illustration, we have reproduced in this case the $e^+e^- \rightarrow 7 \gamma$ cross section.

![Figure 1: Acceptance rates, $A$, defined as the ratio of accepted over generated MC points (times 100), for the VEGAS algorithm in evaluating the total cross section for $e^+e^- \rightarrow n \gamma$, with $n = 1, \ldots, 9$, for five possible choices of ITMX and NCALL, such that their product is approximately equal to $N_{MC} = 10^6$.

Before proceeding to compare the algorithms, one should recall that in VEGAS there exist two parameters, NCALL and ITMX, that determine the actual number of points generated. The first is the (approximate) number of integrand evaluations per iteration whereas the second is the maximum number of the latter. To change one or the other affects the overall performance of the algorithm in various respects. Thus, as a preliminary exercise, we have run VEGAS varying these two parameters: e.g., by taking ITMX = 1, 2, 4, 5, 10 and, consequently, NCALL = $N_{MC}$/ITMX, being $N_{MC} = 10^6$. The outcome is presented in Fig. 1, where we show the acceptance rate, $A$. There, one can first notice the indifference of VEGAS to the choice of NCALL and ITMX for $n \leq 4$, that is, if the dimension

\[\text{As we set the required accuracy to be negative, i.e., ACC < 0, all of them are performed.}\]
the integral, NDIM, is below 7. For \( n \geq 5 \), or equivalently NDIM \( \geq 10 \), if one increases ITMX, the adaptability worsen for high dimensionalities while it improves for low ones. As a compromise between the two tendencies, we will adopt for the reminder of this test the choice ITMX = 4 and NCALL = \( N_{MC}/ITMX \) for any \( n \).

In the case a VEGAS iteration fails to find points above the cuts (as it can happen for very large \( n \)), thus yielding a zero, its contribution to the total estimate of the cross section is discarded altogether.

\[
\sigma(e^+e^- \rightarrow n \gamma) \text{ (nb) at } \sqrt{s} = 100 \text{ GeV}
\]

| \( n \) | Metropolis | VEGAS | RAMBO | \(|\times 10^{-2}\) |
|---|---|---|---|---|
| 2 | 2.66782 ± 0.0029 | 2.664973 ± 0.000050 | 2.66114 ± 0.0023 | 2.66782 ± 0.0029 |
| 3 | 6.34056 ± 0.029 | 6.26009 ± 0.017 | 6.26585 ± 0.014 | 6.34056 ± 0.029 |
| 4 | 6.63656 ± 0.036 | 6.63202 ± 0.050 | 6.67522 ± 0.025 | 6.63656 ± 0.036 |
| 5 | 4.0304 ± 0.034 | 3.94629 ± 0.054 | 3.99786 ± 0.023 | 4.0304 ± 0.034 |
| 6 | 1.49256 ± 0.013 | 1.48609 ± 0.048 | 1.47493 ± 0.010 | 1.49256 ± 0.013 |
| 7 | 3.72003 ± 0.037 | 3.73682 ± 0.26 | 3.63071 ± 0.040 | 3.72003 ± 0.037 |
| 8 | 5.92104 ± 0.072 | 5.51518 ± 0.51 | 5.83508 ± 0.077 | 5.92104 ± 0.072 |
| 9 | 6.43459 ± 0.079 | 5.62617 ± 1.3 | 6.57829 ± 0.21 | 6.43459 ± 0.079 |

| \( n \) | D01EAF | D01GCF | \(|\times 10^{-2}\) |
|---|---|---|---|
| 2 | 2.66510 ± 0.0019 | 2.66493 ± 0.000010 | 2.66510 ± 0.0019 |
| 3 | 6.19822 ± 0.29 | 6.15469 ± 0.031 | 6.19822 ± 0.29 |
| 4 | 6.47451 ± 4.1 | 6.60557 ± 0.13 | 6.47451 ± 4.1 |
| 5 | 5.13410 ± 4.8 | 4.11628 ± 0.45 | 5.13410 ± 4.8 |
| 6 | 11.2745 ± 42. | 1.44837 ± 0.21 | 11.2745 ± 42. |
| 7 | 0.776428 ± 33. | 2.87767 ± 0.64 | 0.776428 ± 33. |
| 8 | 3.56037 ± 385. | 4.93633 ± 2.2 | 3.56037 ± 385. |
| 9 | 59.0009 ± 866. | cannot compute | 59.0009 ± 866. |

| \( E_\gamma = 5 \text{ GeV} \) | \( \cos \theta_\gamma < 0.9 \) |

Table 1: The cross sections and relative errors for \( e^+e^- \rightarrow n \gamma \) at \( \sqrt{s} = 100 \text{ GeV} \), with \( n = 1,...,9 \), as obtained from the five algorithms documented in the text. For VEGAS, the setup ITMX = 4 and NCALL = 250000 was adopted. Several values of MINCLS (see Ref. [16]) were used for D01EAF, but no significant improvement was found compared to the data reported.

\[ ^{11} \text{Note that we have mapped the } n\text{-photon phase space in such a way the the azimuthal angle around the electron/positron beam direction is one of the integration variables. Being the cross section independent of this variable, the phase space integral can be reduced by one dimension and simply multiplied by } 2\pi. \text{ Of course, four of the initial } n^4 \text{ dimensions of the phase space integral are removed by the } \delta\text{-functions associated to the four-momentum conservation between the initial and final states.} \]
In Tab. 1 we present, as function of $n$, the central values and the associated errors produced by the five integrators considered in evaluating the cross sections for $e^+e^- \to n \gamma$ (compare to Tab. 1 of Ref. [14] for $n \leq 7$). (D01GCF cannot compute integrals with more than 20 dimensions, so that the cross section corresponding to $n = 9$ does not appear in the table.) A first obvious result (apart from the shortcomings of D01EAF as $n$ increases) is that whereas VEGAS performs undoubtedly better than Metropolis for small $n$, say, below 4, if $n \geq 4$, Metropolis yields a much more accurate answer. Even RAMBO, a non-adaptive algorithm, excels over VEGAS for large photon multiplicities, though, for $n = 9$, not as well as Metropolis. The error from D01GCF is significantly larger than that for the other algorithms (except D01EAF) for $n \geq 4$, whereas for smaller values it almost achieves the accuracy of VEGAS.

Figure 2: Acceptance rates, $A$ (above), defined as the ratio of accepted over generated MC points (times 100), and relative error, $E$ (below), defined as the ratio of the standard deviation over the average value, for the Metropolis, VEGAS and RAMBO algorithms in evaluating the total cross section for $e^+e^- \to 7 \gamma$, as a function of $N_{MC}$. For VEGAS, the setup ITMX = 4 and NCALL = $N_{MC}/$ITMX was used. (Note the overlapping errors for Metropolis and RAMBO.)
Therefore, for high-dimensionality phase spaces, Metropolis, and \textsc{rambo} as well, seem to be much more accurate than \textsc{vegas}. However, one might well wonder what is the actual number of points used in the evaluation of the integral, as the accuracy of the latter strongly depends upon it. It turns out that the acceptance rate of \textsc{vegas} (recall Fig. 1) is very poor compared to that of Metropolis and \textsc{rambo}, which is about 61(59)[56] \% and 19(10)[4] \% for \( n = 7(8)[9] \), respectively. (In particular, the large difference between the acceptance rates of Metropolis and \textsc{rambo} for the case \( n = 9 \) should explain the much smaller error for the former.) Thus, it is not surprising to see a bigger error in the former. Indeed, if \textsc{vegas} itself is run in non-adaptive mode (i.e., ITMX = 1) its acceptance significantly improves (see again Fig. 1) and the error consequently diminishes (typically halved), still being larger than in Metropolis and \textsc{rambo}, though.

However, in order to show that the higher accuracy for Metropolis, as compared to \textsc{vegas}, for a large number of dimensions is not an artifact due to the specific value adopted for \( N_{\text{MC}} \), we plot in Fig. 2 both the acceptance and the size of the relative error for the two algorithms in calculating, e.g., \( \sigma(e^+e^- \rightarrow 7 \gamma) \), with \( N_{\text{MC}} = 10^6, 10^7 \) and \( 10^8 \) (as usual, ITMX = 4 in \textsc{vegas}). Similarly, we proceed for \textsc{rambo}. One can see that, no matter how many MC points one can dispose of in \textsc{vegas}, both the adaptability and accuracy in Metropolis remain significantly better. The gain for \textsc{vegas} is in the end only appreciable against \textsc{rambo}: Metropolis still stands out as the best choice for large \( n \) values, whatever \( N_{\text{MC}} \) is actually used for the integration. This statement remains true for any choice ITMX = 1, 2, 4, 5, 10 adopted in \textsc{vegas}.

\section{3.2 Mass singularities, multi-channels and negative weights}

The physics concerned with our discussion below can be found in Refs. [13,20]. The process calculated is \( e^+e^- \rightarrow b\bar{b}W^+W^- \), with massive quarks (and gauge bosons, of course), proceeding at tree-level through the 61 Feynman diagrams depicted in Fig. 1 of Refs. [13,20] (again, we assume \( m_e = 0 \)). These include several graph subsets (eight of these were isolated in Ref. [20]), each having a peculiar (non-)resonant structure, so that they can be regarded as separate production modes of an actual multi-channel process. Furthermore, since interference terms exist in the full ME among the various channels, some of the latter can give rise to negative contributions in the integration procedure (the \( T \) weights of Metropolis discussed previously).

For sake of illustration and comparison among the algorithms, rather than generating the total \( e^+e^- \rightarrow b\bar{b}W^+W^- \) cross section in a unique run using \textit{a-priori} weights to choose among the various channels (i.e., a \( \text{à la} \) [1]), we instead perform a separate integration over each of the latter, as they present different challenges.
to the algorithms, see Refs. [19][20]. In general, our approach can be viewed as a preliminary by-hand optimisation of the weights eventually used in a full ME multi-channel run, rather than the automatic one discussed in Ref. [5]. Numerical values used here for the various parameters needed for the calculation are as follows (the reader should not mind their obsolescence, as they are used for illustration purposes):

\[ \sqrt{s} = 300 \text{ GeV}, \ m_t = 145 \text{ GeV}, \ \Gamma_t = 0.78 \text{ GeV}, \ m_b = 5 \text{ GeV}, \ M_H = 120 \text{ GeV}, \ \Gamma_H = 6.9 \text{ MeV}, \ M_Z = 91.1 \text{ GeV}, \ \Gamma_Z = 2.5 \text{ GeV}, \ M_W = 80 \text{ GeV} \]

and \( \Gamma_W = 2.2 \text{ GeV}. \) Note that we do not impose any cuts on the phase space (so that all \( N_{\text{MC}} \) generated points are actually used in the ME evaluations) and we neglect initial state radiation (ISR), thus identifying the partonic energy with that of the collider.

No cuts No ISR

Table 2: Contributions to the total cross section for \( e^+e^- \rightarrow b\bar{b}W^+W^- \) of the eight (non-)resonant channels of Ref. [20], as obtained from the three algorithms documented in the text. For VEGAS, the setup ITMX = 5 and NCALL = 100000 was adopted.

The algorithms chosen for this test are Metropolis, VEGAS and RAMBO. In running RAMBO, we have not set up any special arrangement in dealing with the complicate phase space structure of the various channels [19][20]: we have let the algorithm generate four-momenta and weights and computed the estimate and error of the total cross section as described in the previous Subsection. As for VEGAS, we have adopted here the same mapping of the integration variables described in Ref. [20]. Concerning the Metropolis implementation, the expression in eq. (7) of Subsect. 2.1 was used for computing the cross section. This method is applicable when the ME can be expected to have negative values. Also, the massive phase space volume was calculated beforehand and with insignificant errors. Notice that the \( N_{\text{MC}} \) statistics used here should be taken as representative of a value for which all three algorithms converge to the correct integrals (see Ref. [19][20]). Indeed, if this is augmented,
errors diminish considerably in each case, though the relative performances among Metropolis, VEGAS and RAMBO remain basically unaffected.

The eight terms $T_i$, $i = 1, \ldots, 8$, of eqs. (9)–(16) in Ref. [20], integrated over the full four-particle phase space, are presented in Tab. 2, as obtained by using Metropolis, VEGAS (ITMX = 5 and NCALL = 100000) and RAMBO, with $N_{MC} = 500000$. Here, it definitely is VEGAS to come out best, with second choice Metropolis and last RAMBO. The flaws of the latter should have been expected, as the algorithm is not adaptive so that it suffers from the presence of peaks rising over the phase space. This is particular evident in the $T_7$ channel, which accounts for the very narrow $H \to b\bar{b}$ resonance [20] (recall that the Higgs width is just a few MeV)\footnote{Further notice that, being $M_H < 2 M_W$, the Higgs decay channel $H \to W^+ W^-$ in $T_4$ is not open.}. In fact, when the resonant particles involved have a width of a few GeV (i.e., $t$, $\bar{t}$, $Z$ and $W$), such as in $T_i$ with $i = 2, \ldots, 6$, the accuracy improves, unless two resonances have to be evaluated at once, those from top quark pairs in $T_1$. Here, the error does become very significant (about 10%).

Metropolis behaves better than RAMBO, as its error is always smaller. It deals with single resonances rather satisfactorily for the quite low statistics used (when $i = 4, 7$). No particular problems arise in Metropolis in dealing with negative weights (and rapidly changing interferences) either, i.e., $T_i$ when $i = 2, 3, 5, 6, 8$, as here the typical error does not worsen in comparison to the cases in which the integrand function is definite positive (i.e., $i = 4, 7$). However, Metropolis is no matching to VEGAS, particularly when multiple resonances are present, as in $T_1$.

In the end, the careful mapping performed in VEGAS of all resonances and interferences has paid off. However, one should notice the minimal involvement of the Metropolis implementation in this case, compared to the VEGAS one. In the Metropolis algorithm, there are no phase space Jacobian factors to be accounted for. On the other hand, we have stressed how they can efficiently be used in VEGAS to remove poles arising from the ME. Indeed, we will show in the next Subsection that, if an effort similar to that devoted to VEGAS here is employed for Metropolis as well (in ‘teaching’ to the algorithm the singular structure of the integrand function), then the performance of the latter can match that of the former.

### 3.3 Variable energy, high multiplicity final states and cuts

We dedicate this final Subsection of our numerical analysis to study the process $gg \to b\bar{b}t\bar{t} \to bbbW^+W^- \to bbbjj\ell^\pm\nu_\ell$ (where $j$ represents any light-quark jet and $\ell^\pm/\nu_\ell$ a lepton/neutrino), which was considered in Ref. [21] as a QCD background to a possible charged Higgs discovery channel for the Large Hadron Collider (LHC). Numerical parameters and other inputs used for the runs were declared there.
In this test, there are three specific technical problems associated with the calculation of the total cross section. Firstly, the fact that the CM energy at partonic level is no longer a constant (contrary to the two previous examples): being a hadron-hadron process, two more integrations (in additions to those over the phase space) have to be performed, over the gluon momentum fractions, which evolve according to the PDFs inside the proton. Secondly, the very large number of final state particles, eight in total, which imposes a 21-dimensional integration over the phase space\footnote{One degree of freedom being absorbed into the flat azimuthal integration about the incoming beam direction (see discussion in Subsect. 2.3.3), and already accounting for the PDF convolution.} (beside the presence of various mass singularities, both infrared and resonant poles). Thirdly, the introduction of severe reductions of the original integration region, as we have enforced in our simulations the same acceptance and selection cuts recommended in Ref. \cite{21}, the latter being implemented simply through theta functions\footnote{In fact, it turns out impossible to map the entire phase space in terms of the kinematic quantities whose range is being cut, and not any more efficient to use only one or two of these as integration variables.}. The algorithms used in this example were only two: Metropolis and \textsc{vegas}. The latter uses as usual a careful mapping around the heavy particle resonances, through the variable

$$\phi = \arctan \left( \frac{Q^2 - M^2}{M \Gamma} \right)$$

(13)

(where $M$ and $\Gamma$ represent the natural mass and width of the unstable particle, $t, \bar{t}$ or $W^\pm$, with virtuality $Q^2$), whose derivative is proportional to the resonant propagator itself:

$$d\phi = \frac{M \Gamma}{(Q^2 - M^2)^2 + M^2 \Gamma^2} dQ^2.$$ 

(14)

The setup of the former is as described in Subsect. \[2.3.3\]. This is the most involved implementation of the Metropolis algorithm which was tested. In this case, one needs an approximate ME with known cross section at a certain energy: this was constructed by simply using the two $W$- and the two $t$-resonances. Therefore, the Metropolis approach adopted here can be viewed as the equivalent of the \textsc{vegas} mapping enforced through eqs. (13)–(14). The cross section associated to this auxiliary ME at one energy was calculated numerically beforehand. In the following, we assume the latter to be known with arbitrary small error. In this respect, we should also mention that in our actual ME we have ignored interference effects between the two subsets of Feynman diagrams that only differ in the exchange of the four-momenta and spins between the two $b$-quarks (or, equivalently, the two $b$-antiquarks) in the final state, because of their indistinguishability in the detector, and a minus sign, because of the Fermi-Dirac statistics (in other terms, the Pauli principle). In fact, their effects on the total and differential cross sec-
tions are negligible [21]. Besides, their integration would pose further, unnecessary complications.

\[
\frac{\Delta \sigma}{\sigma (gg \rightarrow X \rightarrow bbbjjj\ell^{\pm}\nu_{\ell})} \,(\%)
\]

| \(\sqrt{s} \,(\text{TeV})\) | Metropolis | VEGAS |
|-----------------|-----------|-------|
| \(X \rightarrow \text{only top-antitop radiation, no PDFs}\) |           |       |
| 0.6             | 1.92      | 0.48  |
| 1.0             | 4.25      | 0.99  |
| 1.4             | 6.88      | 1.52  |
| \(X \rightarrow \text{full ME, no PDFs}\) |           |       |
| 0.6             | 0.77      | 0.32  |
| 1.0             | 2.15      | 0.61  |
| 1.4             | 2.96      | 0.72  |
| \(X \rightarrow \text{full ME, PDFs}\) |           |       |
| \(\sqrt{\tau s}\) | 3.58      | 1.53  |

Table 3: The relative error on several cross sections associated to the process \(gg \rightarrow X \rightarrow bbbjjj\ell^{\pm}\nu_{\ell}\) at \(\sqrt{s} = 14\) TeV, as obtained from the two algorithms documented in the text, each using about \(10^6\) MC points (all passing the default cuts of Ref. [21]). We have verified that actual cross sections (not shown here) are statistically consistent between the two algorithms.

As we have already digressed to some length about the relative ability of the two algorithms to adapt, we make our primary concern in this test that of comparing the size of the errors associated to the integrals in each case. In order to render the comparison consistent, regardless of the actual value of point generated, \(N_{\text{MC}}\), we always compute the integrals for a given statistics in both cases, e.g., \(10^6\) (that is, the latter is the approximate number of MC points that actually pass the cuts). We proceed to obtaining the final result by steps, in order to assess whether one algorithm outperforms the other in some specific task. We start by isolating a gauge-invariant substructure of the original ME, only comprising those diagrams (eight in total) in which the off-shell gluon, \(g^*\), eventually splitting into \(b\bar{b}\) pairs, is emitted by either of the top (anti)quarks, the latter finally decaying semileptonically. Moreover, we fix the partonic CM energy, i.e, \(\sqrt{\tau s}\) = constant, thus removing for the time being the integrations over the gluon PDFs. As the corresponding cross section has little meaning physics-wise, we only plot the relative error as obtained from the two algorithms, e.g., at \(\sqrt{s} = 600, 1000\) and \(1400\) GeV. The upper part of Tab. 3 shows the rates for the simpler subprocess just described, i.e., \(gg \rightarrow t\bar{t} \rightarrow g^*t\bar{t} \rightarrow bbt\bar{t} \rightarrow bbbW^+W^- \rightarrow bbbjjj\ell^{\pm}\nu_{\ell}\). At all energies, VEGAS yields a smaller error than Metropolis, by about a factor of four. Although Metropo-
lis is still outperformed by VEGAS in the size of the relative error of the various integrations, one should notice that the differences between the two algorithms have diminished substantially: compare to the rates in Tab. 2. In both cases, the relative error increases with $\sqrt{\hat{s}}$. In order to understand this effect, it should be recalled that, although the final state particles are jets and leptons (thus with negligible rest mass as compared to the $\sqrt{\hat{s}}$ values used), the two (anti)top resonances involved impose that the cross section would drastically fall to negligible levels if $\sqrt{\hat{s}} \lesssim 2(m_t + m_b)$. Effectively, the volume of the phase space associated with the integration performed at $\sqrt{\hat{s}} = 600 \text{ GeV}$ is much smaller that that spanned when $\sqrt{\hat{s}}$ is $1400 \text{ GeV}$, where the 8-particle phase space can stretch much further away from the $b\bar{b}t\bar{t}$ threshold at $360 \text{ GeV}$. Therefore, one would conclude that the tendency of both integrators to giving smaller errors at lower CM energies is a consequence of the fact that the integrand function fluctuates more at larger $\sqrt{\hat{s}}$.

As a second step of our test, we have introduced the full ME, see Ref. [21], in place of the reduced one considered so far, where by ‘full’ we intend the one obtained by allowing for the attachments of the off-shell $g^* \rightarrow b\bar{b}$ current to the gluon lines too, but with the process still proceeding via the production of two top (anti)top quarks, and without the mentioned interferences. This $2 \rightarrow 8$ ME consists of 36 basic Feynman diagrams. Not to complicate things further, we again express the gluon PDFs through $\delta$-functions centered around one and fix the partonic energy $\sqrt{\hat{s}}$ at the usual three values: 600, 1000 and 1400 GeV. Results are presented in the middle part of Tab. 3. The relative performances of the two algorithms are rather similar to the previous case, though the overall error has diminished at each energy in both Metropolis and VEGAS. This effect is presumably the consequence of the fact that the additional contributions to the ME fill regions of the phase space previously empty, these smoothly interpolating into those typical of the kinematics of gluon emission from (anti)top quarks.

The final step is the integration over the full ME, including the convolution with the PDFs, i.e., $\hat{s} = x_1 x_2 s = \tau s$, with $\sqrt{s} = 14 \text{ TeV}$. In VEGAS, the latter was done by adding the two integrations over the two gluon momentum fractions, i.e., $x_1$ and $x_2$, (so that NDIM $= 21$) and the call to the PDF numerical package. In Metropolis, we have proceeded as follows. One of the integrations over the momentum fractions was performed beforehand. This was done by first changing the momentum fraction variables into the logarithm of the (squared) CM energy and rapidity of the two gluons (as in VEGAS):

$$\frac{dx_1}{x_1} \frac{dx_2}{x_2} = d\ln(x_1 x_2) d\ln \sqrt{\frac{x_1}{x_2}}.$$ 

The rapidity spectrum was then integrated at fixed CM energy, this yielding a distribution in the latter variable only. This was in turn convoluted into the weight-function. The complete integration was finally done by combining the variable
energy and parallel integration methods, as described in Subsect. 2.3.3. The region $400\ \text{GeV} \lesssim \sqrt{s} \lesssim 2\ \text{TeV}$ was chosen, large enough to gather the main contributions to the cross section. From the lower part of Tab. 3 one can see that, even in presence of the complete differential structure of the cross section, VEGAS performs better than Metropolis in terms of accuracy, but the relative size of the error has gone down, to a factor slightly larger than two only. The absolute size is larger than in the previous test for both algorithms, a consequence of the additional dependence upon the gluon PDFs.

As intimated at the end of the previous Subsection, if a similar sort of care is devoted to both algorithms in order to better account for the singular structure of the MEs, one should conclude that, although VEGAS is still better in minimising the accuracy of the integration, Metropolis represents at least a viable alternative. This becomes particularly true if one finally considers that, even in this context, Metropolis displayed a better tendency than VEGAS to adapt in high dimensions and over a reduced phase space, as already seen elsewhere. In other words, the same accuracy can be achieved by the former with much less CPU-time effort than for the latter.

4 Conclusions and outlook

Adaptive MC programs have become an indispensable tool in high energy particle physics, in order to calculate reliably decay and scattering cross sections over multi-dimensional phase spaces. Indeed, as the energy reach of modern particle accelerators grows larger, both the number of particles that can be accommodated in the final state and that of the channels through which they can be produced, increase rapidly. Under these circumstances, it is evident that simple generalisations of well known one-dimensional integration methods are no longer applicable, given the huge number of points that would be needed in order to overcome the high complexity of the integrand functions (let alone the use of analytic methods, if one further considers the need of accounting for non-trivial reductions of the integration volume, because of unavoidable experimental cuts).

Although several algorithms already exist on the market nowadays, which perform their task sufficiently well to have enabled stringent tests between theory and experiments, it is clear that the availability of new implementations is a need never exhausted: if only for cross-checking purposes. For this and other reasons, we have developed several new implementations of an old MC technique: the so-called Metropolis method. Although being another adaptive MC algorithm, it can boast at least one radically different feature with respect to traditional approaches: in the latter, the integration over the phase space takes place over a grid; in the former, it evolves along a path. This discretisation of the integration volume has historically
appealed to the solution of problems in statistical mechanics and Lattice Gauge Theories. However, there is basically no reason why such a technique can not be applied successfully also to the four-momentum phase space of Quantum Field Theories.

As a matter of fact, we have here demonstrated the high potential of the Metropolis method in dealing with realistic problems arising in modern particle physics phenomenology. It not only fulfills the basic criteria of accuracy and efficiency required to any algorithm, no matter the number of dimensions involved in the integration, but it has also been shown to outperform in some cases other, already widely diffused MC programs. Moreover, being its speed matter of no concern at all, the Metropolis algorithm could well be used in (parton level) MC event generators too.

There can certainly be drawbacks in the application of the method. The most important being the need at times of optimising the implementation of the Metropolis algorithm to solve a specific problem, which can require prior knowledge of the behaviour of the integrand function. But even then, the reader should acknowledge that it is becoming more and more rare in numerical simulations that one can afford to rely solely on the ability of whatever algorithm in adapting itself to such subtle effects as interferences, finite particle widths, irreducible backgrounds, etc., as some of our examples should clearly have demonstrated.

We have encoded the various implementations of the Metropolis algorithm discussed in this paper in a C++ program, that we make available to the public upon request. This code makes extensive use of the CLHEP classes\cite{22} for handling Lorentz four-momenta.

Before closing, we will describe two possible improvements that could be considered in the future in order to further increase the efficiency of the Metropolis algorithm in QFT. Both these methods are widely used for conventional statistical physics problems, and shown to be necessary tools in many cases.

The first method relies on the introduction of a fictitious reciprocal temperature, $\beta$. This method has seen two different implementations called ‘simulated tempering’\cite{11} and ‘parallel tempering’\cite{23}. In our case, the phase space would be enlarged with $\beta \in [0, 1]$ as a new parameter, inducing a modified weight-function,

$$w(x, \beta) = w^\beta(x).$$

Clearly, the integration is simpler with $\beta$ close to zero, while we want it instead to be performed at $\beta = 1$. This way of enlarging the phase space allows for round tours into the low-$\beta$ region where the configuration can be updated more freely,

\footnote{The difference between the two lies essentially in the way the configuration space is enlarged by means of $\beta$.}
and thus the correlation length is shorter. This is very much in the same manner as when the total energy, $E_{\text{tot}}$, was used as a free parameter (see Subsect. 2.3.2 of this article). The advantage of instead using $\beta$ is that the efficiency of the method would not be as much dependent on the energy variations of the cross section. In any case, this method should, and could rather easily, be tested also in the case of integrations over a four-momentum phase space.

The other technique that we want to mention is known as the ‘Hybrid Monte Carlo’ method [24]. In this case, derivatives of the weight function are used to move large distances in configuration space, but still avoiding the un-favoured regions where the weight function is small. In many cases, this method has increased the efficiency of the Metropolis algorithm drastically and could very well be unavoidable if much more numerically demanding problems are to be treated in the QFTs of the future. Unfortunately, derivatives of more complicated matrix elements are not available today. It is also at present not clear to the authors how this hybrid MC should be implemented to perform integrations over a four-momentum phase space.

A final, more general remark, is the following. Throughout this article, we have described several implementations of the Metropolis algorithm, all using a stepping procedure designed in such a way that the final state particles are kept on mass-shell. An alternative approach would be to map their four-momenta onto a set of independent variables and perform the random walk in the new phase space. This way, one could benefit from the use of mappings which can cancel the ME singularities (e.g., see eqs. (13) and (14) in Sect. 3.3). A possible implementation of this last strategy is now under consideration.

Appendix: a proof for restricted phase spaces

In this Appendix, we will show that, in case the integration is to be done in a subspace of the original phase space, the $PS_{\text{red}}$ of Subsect. 2.1[16], the Metropolis condition (a) is fulfilled, if for any two points inside $PS_{\text{red}}$, there exists a continuous curve $\Gamma$, which connects the two points and is contained in $PS_{\text{red}}$.

For every point $x$ along $\Gamma$, there is an open disc $D(x, r)$, with radius $r$, which is wholly contained in $PS_{\text{red}}$. First, we show that we can choose a $\delta$, $0 < \delta < r$, so that all points on the surface \( \{ y; |x - y| = \delta \} \) can be reached from $x$ in $n - 1$ steps which are all inside $D$.

Suppose, as before, that $x = \{p_i\}$ and $y = \{p'_i\}$ and let $\Delta_i = p'_i - p_i$. We can now move from $x$ to $y$ in $n - 1$ steps, by transferring the $\Delta_i$ one by one to $p_n$ for $i = 1$ to $i = n - 1$. This will take us through $n - 1$ points: $x = x_0 \rightarrow x_1 \rightarrow \ldots \rightarrow x_{n-1} = y$.

---

[16] Which we assume here to be an open subspace.
[17] With the metric of the Euclidian space of the three-momenta.
Let $d$ be the largest of $|x - x_i|$ in this path. Choose an $a$ such that $0 < a < r/d$ and get a new $\delta' = a\delta$. Then the point $y' \equiv x + a(y - x)$ lies on the corresponding surface and can be reached by a path inside the disc $D$. If $\tilde{y}$ is the point on $\{y; |x - y| = \delta\}$ which gives the largest $\overline{d} = \tilde{d}$ and with $0 < \tilde{a} < r/\overline{d}$, we have that all points in $S = \{y; |x - y| = \tilde{a}\delta\}$ can be reached in a finite number of steps, which are all contained in $D$.

A point where $\Gamma$ crosses $S$ has a finite distance $(\tilde{a}\delta)$ to $x$ and it can then be reached with a finite number of steps, all inside $PS_{\text{red}}$. In this way, starting from any point in $PS_{\text{red}}$, any other point can be reached with a finite number of steps inside $PS_{\text{red}}$, by taking finite steps along the corresponding $\Gamma$. This concludes our proof.

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The Metropolis algorithm for on-shell four-momentum phase space: Erratum

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Abstract

A proof presented in the original paper was incorrect. We outline here an alternative procedure.
The new proof

One of the conditions required to the stepping procedure implemented in the Metropolis algorithm, as described in Ref. [1] (point (a) in Sect. 2.1), was that any point \( \{ p'_{i} \} \) in the \( n \)-particle phase space can be reached from any other point \( \{ p_{i} \} \) in a finite number of steps. The proof in the main article relies on the false statement that, for any two on-mass-shell particles with four-momenta \( p_{1} \) and \( p_{2} \), the whole of the surface of conserved \( p_{1} + p_{2} \) can be reached by the identical particles by rotating them in their centre-of-mass (CM) frame. This is however not true, because it would in general be possible to transfer a four-momentum which conserves \( p_{1} + p_{2} \) but puts one or both particles out of the mass-shell. (The rotation procedure itself, in contrast, does preserve the on-mass-shell condition). Below we present a correct proof of the above statement.

It is clear that the whole of the two particle phase space can be reached in a single step, so let us assume that the number of particles (\( n \)) is at least three. We will later on show that it is possible to move any particle (e.g., the \( n \):th), from its original four-momentum \( p_{n} \) to the final one \( p'_{n} \) in a finite number of steps, by exchanging some momentum with the other particles. This procedure will change the other four-momenta to new values \( \{ p''_{i} \} \). The rest of the problem is then to move these to their final values \( \{ p'_{i} \} \). For \( (n - 1) = 2 \), this can be accomplished in one step. For \( n > 3 \), we can move the \( (n - 1) \):th four-momentum to its final value \( p'_{n-1} \), and so on.

Let us first discuss what four-momenta are possible for a given particle, in the case of unrestricted phase space. Consider again the \( n \):th particle, and let \( s \) be the total invariant energy squared, \( s_{n-1} \) be the energy squared of the system of all the other particles and let \( m_{n} \) be the mass of the \( n \):th particle. In the CM frame, the magnitude of the three-momentum of the \( n \):th particle is given by\(^1\)

\[
P_{n} = \frac{1}{2\sqrt{s}} \sqrt{\lambda(s_{n-1}, m^{2}_{n}, s)},
\]

with

\[
\lambda(a, b, c) = a^{2} + b^{2} + c^{2} - 2ab - 2bc - 2ca,
\]

and it can have any direction. Depending on the value of \( s_{n-1} \), \( P_{n} \) can have any value between 0 (for \( s_{n-1} = (\sqrt{s} - m_{n})^{2} \)) and its maximum, \( P_{n}^{\text{max}} \), which occurs at \( s_{n-1} = (\sum_{i=1}^{n-1} m_{i})^{2} \) (the minimal value of \( s_{n-1} \)).

The four-momentum \( p_{n} \) is, from its mass-shell condition, restricted to a three-dimensional sub-space. We will now show that, in case \( P_{n} \) is smaller that its maximal value, there exists a three-dimensional on-mass-shell neighbourhood of

\(^1\)Hereafter, we use \( P \) to indicate the magnitude of a momentum in the CM frame and \( p \) to denote a four-vector in any frame.
in which any point can be reached in two steps, by exchanging momentum with two other particles (denoted below by \(p_1\) and \(p_2\)).

Let \(k_1\) denote the exchanged four-momentum from \(p_1\) to \(p_n\). Our condition for the exchanged momentum is that it keeps both of the particles on their respective mass-shell. Consequently, with \(p_n' = p_n + k_1\) we have \(p_n'^2 = p_n^2 = p_n^2 + k_1^2 + 2k_1p_n \iff k_1^2 = -2k_1p_n\). Similarly, we have the condition \(k_1^2 = 2k_1p_1\), in order to keep \(p_1\) on the mass-shell. These two conditions restrict \(k_1\) to lie on a two-dimensional surface (corresponding to the two rotational degrees of freedom in the CM frame of \(p_n\) and \(p_1\)). We will now show that two particles \(p_1\) and \(p_2\) can be chosen so that the corresponding infinitesimal four-momentum transfers \(\epsilon k_1\) and \(\epsilon k_2\) \((\epsilon \to 0)\) to \(p_n\) are such that \(k = \epsilon k_1 + \epsilon k_2\) has three degrees of freedom. This implies that \(p_n + k\) (for a finite \(k\)) covers an open on-mass-shell neighbourhood of \(p_n\). In the limit \(\epsilon \to 0\), the on-shell conditions impose

\[
\begin{align*}
  p_n k_1 & = 0, \\
  p_n k_2 & = 0, \\
  p_1 k_1 & = 0, \\
  p_2 k_2 & = 0.
\end{align*}
\]

Under such conditions, the four-vectors \(k_i\) are restricted to lie in two-dimensional planes. The vector \(k\) will then have more than two degrees of freedom, unless the planes for \(k_1\) and \(k_2\) coincide. This would in turn imply that the four-momenta \(p_1\) and \(p_2\) are linearly dependent, that is, one can write \(p_1 = ap_2\) for a number \(a\). Consequently, it is enough to show that there exist two other particles such that their four-momenta are not proportional. This condition is equivalent to say that \(P_n\), as was assumed before, is smaller than its maximal value.

To demonstrate this statement, we will show that \(s_{n-1}\) reaches its minimum if and only if all \(n - 1\) four-momenta are proportional to each other, that is, there are numbers \(a_{ij}\) so that one can write \(p_i = a_{ij}p_j\), for any \(i, j \leq n - 1\). This is well known in case all particles are mass-less \((s_{n-1} = 0)\). In case any of them has a mass, one can boost the entire system to the rest frame of such a particle. The minimal value of \(s_{n-1}\) is then reached if all particles have zero three-momentum in the new frame.

This completes the proof that, in case \(P_n < P_n^{\max}\), there is a three-dimensional neighbourhood of \(p_n\) which can be reached in two steps. From this, we draw the conclusion that the final point \(p_n'\) can be reached in a finite number of steps, in case both \(P_n\) and \(P_n'\) are smaller than the maximum. If this was not the case, then there would exist a four-momentum \(p''\), with \(P'' < P_n^{\max}\), which \(p_n\) can come arbitrarily close to, but never reach. But this contradicts the fact that a neighbourhood of \(p''\) is reachable from \(p''\) (and vice versa).

The final step is to show that it is always possible (in case \(n > 2\)) to move from
a point with $P_n = P_{n}^{\text{max}}$ to another point with $P'_n < P_{n}^{\text{max}}$. This follows from the condition $p_i = a_{ij} p_j$, that leaves one degree of freedom for the four-momentum of one of the particles, for fixed values of the others. Since the four-momentum transfer $k$ has two degrees of freedom, one can, in one step, violate the proportionality condition above, with the consequence that $P'_n < P_{n}^{\text{max}}$.

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