

Algorithms for numerically stable scattering amplitudes

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The numerically stable evaluation of scattering matrix elements near the infrared limit of gauge theories is of great importance for the success of collider physics experiments. We present a novel algorithm that utilizes double-precision arithmetic and reaches higher precision than a naive quadruple-precision implementation at smaller computational cost. The method is based on physics-driven modifications to propagators, vertices, and external polarizations.

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Introductions. During the past decades, particle physics experiments have explored the structure of matter and its interactions at an unprecedented pace and precision. We owe much of this scientific progress to the development of particle colliders [1]. The physics program at collider experiments depends critically on theoretical predictions based on the Standard Model of particle physics, which are typically obtained using perturbation theory [2].

At higher orders in the perturbative expansion, scattering matrix elements develop infrared singularities that arise from long-distance interactions between degenerate asymptotic states [3]. These infrared singularities lead to enormous complications in numerical calculations that rely on Monte Carlo methods for the integration over phase space. They have become particularly problematic in the context of semiautomated computations at higher order in QCD, which are needed to realize the full physics potential of the Large Hadron Collider [4,5]. At the next-to-leading order, calculations can be performed with the help of generic infrared subtraction methods [6]. A similar automation at the next-to-next-to-leading order in QCD seems within reach [5]. All existing methods do, however, rely on the cancellation between real-emission matrix elements and their corresponding approximations in the soft and collinear limits [7,8]. Approaching these limits, the finite remainder can only be computed reliably if both the matrix elements and their approximations can be evaluated at high numerical accuracy *individually*.

It is often assumed that numerical stability issues in the computation of matrix elements are best addressed with

the help of multiple-precision arithmetic. In this Letter, we will show that this is neither necessary nor sufficient. We propose a novel method that is computationally more efficient and also offers the opportunity to probe the deep infrared region through a suitable reformulation of the relevant components of tree-level matrix elements. While the details of a numerical implementation can be quite involved, the basic idea behind the method is simple: We express every part of the amplitude in terms of large and small components of four-momenta. Quantities that become parametrically small in the infrared limits appear in most cases in the form of ratios of the small over the large momentum components, and such ratios can always be evaluated reliably. This is in stark contrast to a naive multiple-precision computation, where small quantities typically emerge as the difference between components of four-momenta that are individually large. At no point in the calculation does our new method involve any approximations. All expressions remain exact to the given order in perturbation theory.

Stability problems and solutions. Numerical imprecisions in tree-level matrix elements arise from multiple sources. The one that is most easily understood is the denominator of propagators in momentum space. For massless particles, it contains terms of the form $1 - \cos \theta$, which originate in the retarded Green's functions of the theory. In this context, θ is the opening angle between the momentum of the particle emitting a gauge field quantum and the momentum of the emission. Whether using Feynman graphs or a recursive algorithm such as the Berends-Giele method [9], we need to find a numerically stable algorithm to compute such terms when $\cos \theta \approx 1$. This is relatively straightforward. The numerators of Feynman diagrams, which arise from the spin dependence of the interactions, are harder to control. There are often intricate cancellations among different graphs, which are difficult to achieve numerically.

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To solve this problem, we will propose convenient expressions for the vertex factors and external wave functions and make use of a physical gauge that suppresses interferences in the collinear limits [10].

Scalar products and light-cone momenta: We begin by discussing a numerically stable algorithm to compute the invariant mass of a momentum vector $q = p + k$, which is given by $q^2 = p^2 + k^2 + 2pk$. The key idea is to represent each four-momentum in the numerical calculation as a five-vector, with the fifth component being the virtuality. If this virtuality is known to high precision, the task of finding q^2 reduces to a computation of the scalar product, $2pk$. In anticipation of the expressions needed to evaluate vertex factors involving vector boson currents, we will discuss the most general case of complex four-momenta. The scalar product can be rewritten as

$$2pk = 2p_0k_0 \left[1 - \frac{\bar{p} \bar{k}}{p_0k_0} \right] + 2\bar{p} \bar{k} (1 - \vec{v}_p \vec{v}_k), \quad (1)$$

where

$$\vec{v}_p = \frac{\vec{p}}{\bar{p}}, \quad \text{and} \quad \vec{v}_k = \frac{\vec{k}}{\bar{k}}. \quad (2)$$

The signed magnitudes of the momenta are defined as

$$\bar{p} = p_0 \sqrt{1 - \mu_p^2}, \quad \text{and} \quad \bar{k} = k_0 \sqrt{1 - \mu_k^2}, \quad (3)$$

where

$$\mu_p^2 = \frac{p^2}{p_0^2}, \quad \text{and} \quad \mu_k^2 = \frac{k^2}{k_0^2}. \quad (4)$$

The solutions of the square roots are taken such that the real part is maximized. Evaluating Eq. (3) in terms of μ_p^2 and μ_k^2 ensures that the velocities remain precise for (near) on-shell momenta. The difference $1 - \vec{v}_p \vec{v}_k$ leads to large cancellations at small angles, which is one of the problems we aim to address. A numerically stable computation can be performed with the help of the identity [11]

$$2(1 - \vec{v}_p \vec{v}_k) = (\vec{v}_p - \vec{v}_k)^2. \quad (5)$$

We are left to evaluate the difference in the square bracket of Eq. (1) as accurately as possible. This is achieved with the help of the following identity, again making use of the numerical stability of μ_p^2 and μ_k^2 ,

$$1 - \frac{\bar{p} \bar{k}}{p_0k_0} = \frac{\mu_p^2 + \mu_k^2 - \mu_p^2 \mu_k^2}{1 + \sqrt{1 - \mu_p^2} \sqrt{1 - \mu_k^2}}. \quad (6)$$

In both vertices and propagators we often encounter terms of the form $p_{\pm} = p_0 \pm p_z$. In configurations with momenta collinear to the z direction, the evaluation of such expressions necessitates a reformulation in terms of large and small components. This can be achieved using the following relation:

$$p_{\pm} = \begin{cases} p_0 \pm p_z & \text{if } |p_0 \pm p_z|^2 > |p_0 \mp p_z|^2 \\ & \text{or } |p_z|^2 < |p_{\perp}|^2 \\ \frac{p^2 + p_{\perp}^2}{p_0 \mp p_z} & \text{else} \end{cases}. \quad (7)$$

The condition $|p_z|^2 < |p_{\perp}|^2$ is particularly relevant for the polarization vectors that will be introduced in Eq. (10). It is always fulfilled in the initial-state collinear regions.

In the deep infrared region of final-state collinear sectors of the phase space, it is not possible to store external momentum configurations at sufficient precision to allow for the reliable extraction of transverse or antiparallel components relevant to collinear splittings. These components and the related scalar invariants must be obtained from a phase-space generator that computes them directly in terms of the integration variables. Such generators can be constructed based on any collinear phase-space parametrization, for example [6]. A convenient method for next-to-next-to-leading order (NNLO) calculations was introduced in [12]. The Supplemental Material to this article [13] discusses how it is used in our numerical tests. A high-precision evaluation of the matrix element then requires as input not only the momenta of the individual particles, but also their difference to the collinear direction and the invariants in the collinear sector.

Wave functions of external states: The numerical stability of the external wave functions and their products with vertex factors often plays a key role in numerical computations. It is particularly important in initial- and final-state collinearly enhanced regions. The spinors of external fermions are typically constructed using the Weyl representation [14]

$$\begin{aligned} \chi_+(p) &= \begin{pmatrix} \sqrt{p_+} \\ \sqrt{p_-} e^{i\phi_p} \end{pmatrix}, \\ \chi_-(p) &= \begin{pmatrix} \sqrt{p_-} e^{-i\phi_p} \\ -\sqrt{p_+} \end{pmatrix}. \end{aligned} \quad (8)$$

These expressions are evaluated in a numerically stable fashion in a straightforward manner, by using Eq. (7) to compute the light-cone momenta p_+ and p_- . The polarization vectors pose a slightly more difficult problem, due to their gauge dependence. In the helicity formalism [15], they contain a longitudinal component, which becomes problematic if the angle between the gauge

vector¹ and the momentum is small. This can be made explicit by assuming a gauge vector of $e_\pm^\mu = (1, 0, 0, \pm 1)$, in which case the polarization vector for helicity λ is given by

$$\epsilon_\lambda^\mu(p, e_\pm) = \pm e^{-i\lambda\phi_p} \left[\frac{p^\pm}{\sqrt{2p^+p^-}} e_\pm^\mu + \frac{e^{\mp i\lambda\phi_p}}{\sqrt{2}} (e_x^\mu \pm i\lambda e_y^\mu) \right], \quad (9)$$

with $e_x^\mu = (0, 1, 0, 0)$, and $e_y^\mu = (0, 0, 1, 0)$. One finds that the component along $e_\pm^\mu$ diverges as $\sqrt{p^\pm/p^\mp}$. It is of course possible to remove this artifact by using a gauge vector q with $(\vec{p} \cdot \vec{q})/(p_0 q_0) < 0$. Nevertheless, we propose a different definition based on real-valued three-vectors, due to its convenient numerical and analytical properties

$$\begin{aligned} \epsilon_1^\mu(p) &= \left(0, \frac{(\vec{n} \cdot \vec{p})\vec{p} - (p_0^2 - p^2)\vec{n}}{\sqrt{\vec{n}^2(p_0^2 - p^2) - (\vec{n} \cdot \vec{p})^2 \sqrt{p_0^2 - p^2}}} \right), \\ \epsilon_2^\mu(p) &= \left(0, \frac{\vec{n} \times \vec{p}}{\sqrt{\vec{n}^2(p_0^2 - p^2) - (\vec{n} \cdot \vec{p})^2}} \right), \end{aligned} \quad (10)$$

where $\vec{n}$ is $\vec{e}_x$, $\vec{e}_y$, or $\vec{e}_z$, depending on whether the largest component of the momentum is in the x , y , or z direction. These real-valued polarizations can be used to define circular polarizations as $\epsilon_\pm^\mu(p) = (\epsilon_1^\mu(p) \pm i\epsilon_2^\mu(p))/\sqrt{2}$.

Vertices and propagators: When the individual components of a polarization vector are large compared to its virtuality, it becomes necessary to track the virtuality as an independent variable in the calculation. Scalar products with other currents are then evaluated using Eq. (1). Similarly, vertex factors involving light-cone momentum fractions should be computed using Eq. (7). Vertices involving fermions and fermion propagators are evaluated in the same fashion.

The computation of off-shell gluon currents [9] in the collinear region of phase space requires special methods in order to avoid numerical instabilities. Consider a pair of on-shell gluons with momenta p_a^μ and p_b^μ and polarization vectors ϵ_a^μ and ϵ_b^μ . The space-time-dependent part of the corresponding two-particle current is generated by the triple-gluon vertex as follows:

$$\begin{aligned} \epsilon_a^\mu \epsilon_b^\nu \Gamma_{\mu\nu\rho}(p_a, p_b, -p_{ab}) &= (\epsilon_a \epsilon_b)(p_a - p_b)^\rho + (2p_b \epsilon_a) \epsilon_b^\rho \\ &\quad - (2p_a \epsilon_b) \epsilon_a^\rho, \end{aligned} \quad (11)$$

where $p_{ab} = p_a + p_b$. In the collinear limit $p_a \parallel p_b$, the last two terms are nearly transverse, because they are

¹In the helicity formalism, the polarization vectors are given by $\epsilon_\pm^\mu(p, q) = \pm \langle q^\mp | \gamma^\mu | p^\mp \rangle / (\sqrt{2} \langle q^\mp | p^\pm \rangle)$, with q^μ the gauge vector.

proportional to the one-particle currents. While formally transverse to p_{ab} , the first term, in fact, has a large longitudinal component that can be made explicit in a Sudakov decomposition [16]

$$\begin{aligned} p_a^\mu &= z_a \tilde{p}_{ab}^\mu + \frac{k_\perp^2 + p_a^2}{z_a 2 \tilde{p}_{ab} n} n^\mu - k_\perp^\mu, \\ p_b^\mu &= z_b \tilde{p}_{ab}^\mu + \frac{k_\perp^2 + p_b^2}{z_b 2 \tilde{p}_{ab} n} n^\mu + k_\perp^\mu. \end{aligned} \quad (12)$$

Here, n is an auxiliary, lightlike vector that is linearly independent of the gluon momenta, and we have defined $\tilde{p}_{ab}^\mu = p_{ab}^\mu - p_{ab}^2/(2p_{ab}n)n^\mu$, as well as $k_\perp^2 = -k_\perp^2$. For practical applications, we choose $n = (\sqrt{\tilde{p}_{ab}^2}, -\vec{p}_{ab})$. To improve the numerical stability of Eq. (11), we perform the calculation in a lightlike axial gauge, which is particularly suitable for collinear parton evolution [10]. In this gauge, the gluon polarization tensor reads

$$d^{\mu\nu}(p_{ab}, n) = -g^{\mu\nu} + \frac{p_{ab}^\mu n^\nu + n^\mu p_{ab}^\nu}{p_{ab} n}. \quad (13)$$

Multiplication by $(p_a - p_b)^\mu$ from the first term of Eq. (11) yields the simple expression

$$d_\rho^\mu(p_{ab}, n)(p_a - p_b)^\rho = 2k_\perp^\mu + (z_a - z_b) \frac{p_{ab}^2}{p_{ab} n} n^\mu. \quad (14)$$

Upon using the dedicated phase-space generator discussed earlier to parametrize the collinear limit, the values of $k_\perp^\mu$ and p_{ab}^2 are known to high precision.

Similar to the gluon currents, quark currents require a dedicated treatment in the collinear limit. Consider the product of propagator numerator and vertex factor for an on-shell quark a coupling to an on-shell gluon b ,

$$(\not{p}_a + \not{p}_b) \not{\epsilon}_b u_a = (2p_a \epsilon_b) u_a - i \sigma_{\mu\nu} p_b^\mu \epsilon_b^\nu u_a. \quad (15)$$

The scalar interaction term can be evaluated using the methods described above. The magnetic term creates numerical instabilities of a different type. Using the Weyl representation of the γ matrices, and the circular polarizations based on Eq. (10), we obtain

$$\begin{aligned} \frac{\sigma_{\mu\nu} p_b^\mu \epsilon_{b,+}^\nu}{\sqrt{2}|p_{b\perp}|} &= \left(\begin{array}{c|cc} 0 & & 0 \\ \hline & 1 & -p_{b\perp}^+/p_{b\perp} \\ 0 & p_{b\perp}/p_b^+ & -1 \end{array} \right), \\ \frac{\sigma_{\mu\nu} p_b^\mu \epsilon_{b,-}^\nu}{\sqrt{2}|p_{b\perp}|} &= \left(\begin{array}{cc|c} -1 & -p_{b\perp}^*/p_b^+ & \\ \hline p_b^+/p_{b\perp}^* & 1 & 0 \\ 0 & 0 & 0 \end{array} \right) \end{aligned} \quad (16)$$

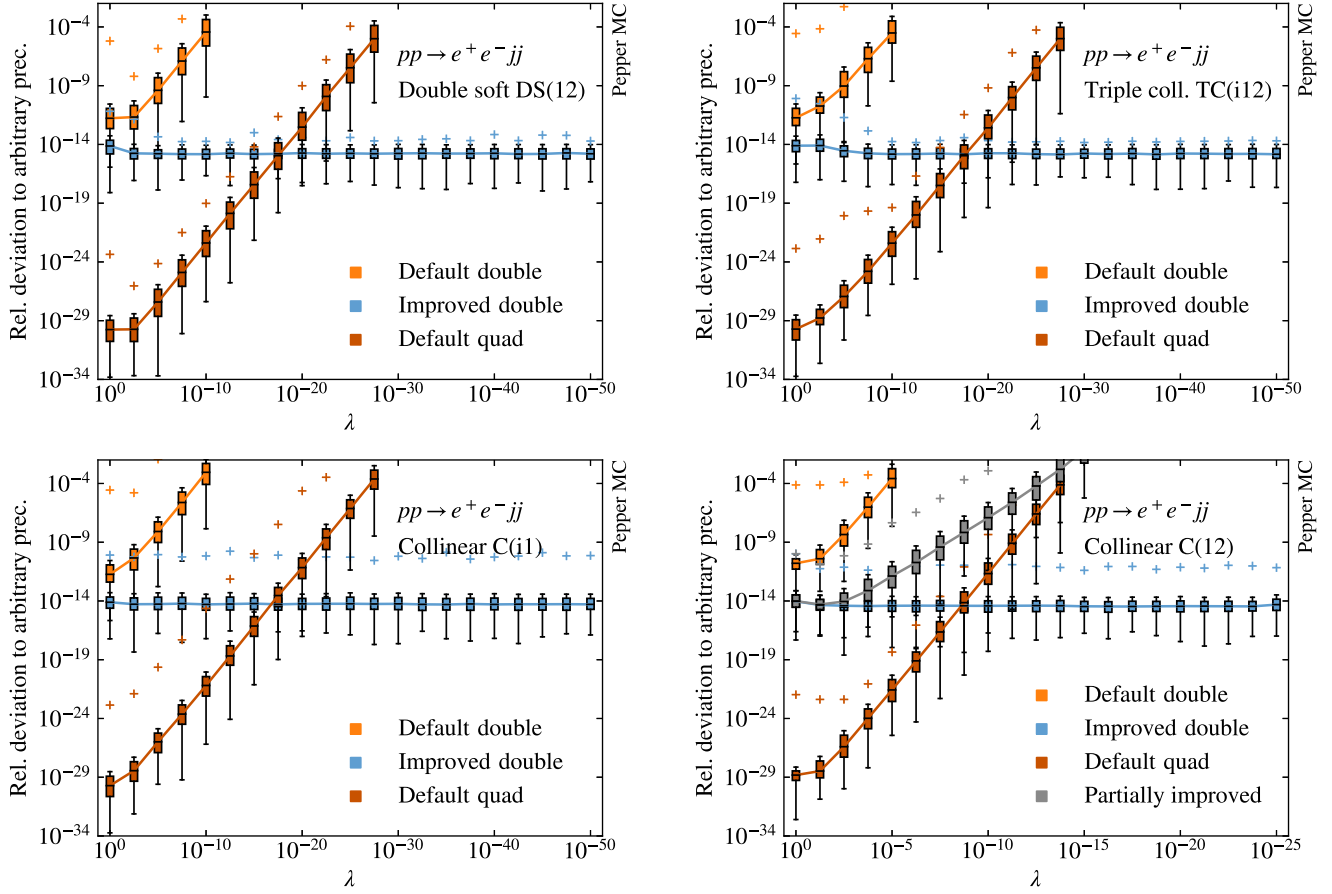


FIG. 1. Relative precision of the matrix-element computation as a function of the scaling parameter λ (see Supplemental Material [13]), in the double-soft (top left), triple-collinear (top right), initial-state double-collinear (bottom left), and final-state double-collinear (bottom right) limit. We compare a naive double-precision (orange), naive quadruple-precision (red), and improved double-precision (blue) implementation. The box plots are obtained from 10^4 phase-space trajectories constructed as described in Supplemental Material [13]. The boxes show the quartiles of the distribution, the whiskers indicate $3/2$ of the interquartile range, and the crosses mark the maximum values. The grey distribution shows the improvements obtained in final-state collinear regions without a Sudakov decomposition of the spin-dependent part of interaction vertices.

In the exact collinear limit, $p_a = z_a p_{ab}$, $p_b = z_b p_{ab}$, the products of these matrices and the Dirac spinors derived from Eq. (8) vanish. Numerically precise results in final-state collinear regions can therefore only be obtained by expressing $\sigma_{\mu\nu} p_b^\mu \epsilon_b^\nu u_a$ in terms of Sudakov variables similar to Eq. (12), but separating the transverse momentum $k_\perp$ into a component $k_\perp^+$, which is parallel to the z axis, and a remainder in the transverse plane.

Example application: LHC physics. We demonstrate the utility of our method using tree-level matrix elements for Drell-Yan lepton-pair production in association with two jets. The reference value is obtained from a calculation in arbitrary-precision arithmetic with 256 significant digits, using the MP++ library [17]. Figure 1 compares the achieved precision relative to the target from this implementation in the double-soft, triple-collinear, and double-collinear limits. We adopt the scaling procedure described in

Supplemental Material of this article [13], which relies on the phase-space parametrization of [12].

In order to gauge the numerical stability of our algorithms in a practical calculation, we perform a computation of the $u\bar{u}$ contribution to the NNLO correction, $\delta\sigma_{\text{NNLO}}$, in Drell-Yan lepton-pair production at the LHC at $\sqrt{s} = 13$ TeV. We use the PDF4LHC15+LUXqed NNLO PDF set [18] and the corresponding definition of the strong coupling. The electroweak parameters are defined as $\sin^2\theta_W = 0.2223$ and $\alpha = 1/128.89$. We set $m_Z = 91.1876$ GeV and $\Gamma_Z = 2.4952$ GeV. The final-state electrons are required to fulfill $66 \text{ GeV} \leq m_{e^+e^-} \leq 116 \text{ GeV}$. Table I shows the results for $\delta\sigma_{\text{NNLO}}$ in the $u\bar{u}$ channel, computed using jetiness slicing [19]. The results labeled “BG recursion” are obtained from a Berends-Giele recursion, using a combination of MCFM [20] and PEPPER [21,22]. All other results use analytic matrix elements (ME), and stem from MCFM. The uncertainty on the results is driven by the subtracted real-emission corrections, for

TABLE I. Contribution of the $u\bar{u}$ initial state to the NNLO correction in $pp \rightarrow e^+e^-$ at $\sqrt{s} = 13$ TeV. See the main text for details.

τ_{cut}	$\delta\sigma_{\text{NNLO}}(u\bar{u} \rightarrow e^+e^- + X)$ (pb)		
	Naive double	Improved double	
		Analytic ME	BG recursion
10^{-2}	28.11(5)	28.12(5)	28.10(7)
10^{-3}	27.4(3)	27.0(1)	27.0(1)
10^{-4}	27.2(4)	27.4(3)	27.0(3)
10^{-5}	...	27.2(9)	27.1(8)
10^{-6}	...	27.7(18)	27.4(16)

which we employ the techniques described before, both in the real-emission matrix element and in all associated infrared counterterms. The calculation reported in Table I should be independent of the parameter τ_{cut} in the limit $\tau_{\text{cut}} \rightarrow 0$ and, in practice, one must choose a value of τ_{cut} that is deemed to be in the asymptotic region. The naive double-precision implementation fails below $\tau_{\text{cut}} \approx 10^{-4}$, leaving only two data points to support this assertion. It is therefore not clear whether the result is correct. The improved implementation remains usable down to $\tau_{\text{cut}} \approx 10^{-6}$, and its results demonstrate that the asymptotic region has indeed been reached. The total additional computing time expended in our unoptimized code is 5% for MCFM, and 80% for MCFM+PEPPER. We expect a reduction of this overhead in an optimized implementation.

Conclusions. This letter discussed a simple set of physics-driven algorithms to stabilize the computation of tree-level matrix elements needed for precision physics at colliders. The methods are applicable to both analytically computed matrix elements and fully numerical approaches. We have presented example numerical results and demonstrated the utility of the technique for precision physics. In view of the increased statistics and reduced experimental systematics in the upcoming high-luminosity phase of the Large Hadron Collider, the improvements discussed here will be of utmost importance for the extraction of Standard Model parameters from experimental measurements.

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