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Two-Loop Four-Gluon Amplitudes with the Numerical Unitarity Method

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We present the first numerical computation of two-loop amplitudes based on the unitarity method. As a proof of principle, we compute the four-gluon process in the leading-color approximation. We discuss the new method, analyze its numerical properties and apply it to reconstruct the analytic form of the amplitudes. The numerical method is universal, and can be automated to provide multi-scale two-loop computations for phenomenologically relevant signatures at hadron colliders.

The experiments at the Large Hadron Collider (LHC) at CERN are entering a new phase in which observables will be studied with relative errors of the order of a few percent. Discoveries through precision measurements require an equal or better control over the theoretical uncertainties of predictions from the Standard Model of particle physics. A central bottleneck to obtaining such predictions is the complexity of computing quantum corrections. We demonstrate a new, automatable algorithm for computing two-loop corrections in QCD based on the established unitarity method. In particular we focus on the numerical variant of the method which has proven valuable for dealing with multi-scale problems. In addition to the flexibility of this approach, the geometric nature of our method simplifies intermediate computational steps and promises good numerical behavior.

As a proof of principle of the new method we recompute the leading-color contributions to the two-loop gluon-gluon scattering amplitudes [1, 2]. This process exposes much of the complexity of two-loop scattering amplitudes in QCD, including their universal infrared and ultraviolet behavior. The expressions in ref. [2] have been obtained using the analytic variant of the unitarity method [3] which constructs scattering amplitudes from their unitarity and analytic properties. This method has been applied to a number of one-loop computations for the LHC, and is the method of choice in formal research on scattering amplitudes in supersymmetric theories. In QCD, at two-loop level, the lack of (super)symmetry and the need for an infrared and ultraviolet regulator pose further challenges due to the appearance of one-loop sub divergences. Nevertheless, analytic computations of fiveand six-gluon amplitudes [4] have recently become available, albeit for constrained helicity configurations. Numerical variants of the unitarity approach at one-loop level [5–8] have by now provided a large number of phenomenologically relevant predictions for the LHC. The

flexibility of the numerical unitarity method in combination with its good numerical stability motivate us to extend it to multi-loop amplitudes. The algorithm which we put forward generalizes the one-loop approach in a non-trivial way, as the two-loop variant requires additional geometric input [9]. Being automatable and less susceptible to the complexity of analytic multi-scale computations, our approach has the potential to mirror the successes found at one-loop level. In addition, analytic expressions can be efficiently reconstructed from a numerical algorithm [10].

In this letter, we present the first numerical computation of two-loop QCD amplitudes with the unitarity method. We focus on the two-loop four-gluon amplitudes which we validate by comparing with known results [2]. Although the approach applies as well to sub-leading color contributions, for simplicity we omit non-planar diagrams as well as closed fermion loops. First, we set up the equations necessary for a hierarchical extraction of an amplitude's integrand [11]. Second, we decompose integrands of massless four-point amplitudes into master integrals and surface terms, extending the results of [9]. Third, we describe our numerical implementation and the linear algebra techniques employed to compute coefficients for fixed values of the dimensional regulator. Subsequently, we reconstruct the functional form of the regulator dependence and obtain explicit numerical results. Finally, we discuss numerical reconstruction of the analytic amplitude and give our conclusions.

Numerical Unitarity Method. We apply a variant of the unitarity method suitable for analytic and numerical computations which generalizes one-loop methods to higher loop orders. For more details of our approach we refer the reader to ref. [11]. We start with an ansatz for the integrand $\mathcal{A}(\ell_l)$ of a two-loop amplitude [9],

$$\mathcal{A}(\ell_l) = \sum_{\Gamma \in \Delta} \sum_{i \in M_{\Gamma} \cup S_{\Gamma}} \frac{c_{\Gamma,i} m_{\Gamma,i}(\ell_l)}{\prod_{j \in P_{\Gamma}} \rho_j}, \qquad (1)$$

(~)

where Δ denotes the set of two-loop diagrams which specify the possible propagator structures of the amplitude. In fig. 1 we show the set Δ corresponding to planar two-loop four-point massless amplitudes in the leadingcolor approximation. The set of diagrams Δ is organized hierarchically with the partial ordering $\Gamma_1 > \Gamma_2$ if $P_{\Gamma_1} \supset P_{\Gamma_2}$, i.e., if the diagram Γ_2 (a descendant) is obtained from Γ_1 (an ancestor) by removing one or more propagators. Here P_{Γ} denotes the set of propagators associated to diagram Γ . The loop momenta are denoted by $\ell_l, l = 1, 2$ and inverse propagators by ρ_i . The numerators span the full set of independent numerator terms [12] and are restricted by power counting. For each diagram, the set M_{Γ} specifies numerators associated to master integrals and S_{Γ} the set of surface terms (i.e., terms that integrate to zero) necessary to fully parameterize the numerators. The $m_{\Gamma,i}(\ell_l)$ are polynomials in ℓ_l . We work in dimensional regularization such that these, as well as the coefficient functions $c_{\Gamma,i}$, depend on the loop-momentum dimension $D = 4 - 2\epsilon$. Dependence on external kinematics is implicit. For simplicity we focus on leading-color (planar) contributions and consider only gluons in the loops. The remaining non-planar diagrams and fermion contributions to this process can be treated in a similar manner, and we leave this for future studies.



FIG. 1: The hierarchy of propagator structures for planar four-point two-loop gluon amplitude. Only topologically inequivalent structures are shown.

The physical scattering amplitude is obtained in terms of master integrals $I_{\Gamma,i}$,

$$\mathcal{A} = \sum_{\Gamma \in \Delta} \sum_{i \in M_{\Gamma}} c_{\Gamma,i} I_{\Gamma,i}, \qquad (2)$$

as surface terms drop out from eq. (1) after integration. At this stage, we only need to compute the coefficient functions $c_{\Gamma,i}$. In generalized unitarity, they are determined by solving the linear system of equations (1) for values of the loop momenta ℓ_l^{Γ} for which the internal particles go on-shell, $\rho_j \to 0$ for all $j \in P_{\Gamma}$. For the leading terms in this limit [11], putting the ansatz (1) and factorization limits together we obtain

$$\sum_{\text{states}} \prod_{i \in T_{\Gamma}} \mathcal{A}_{i}^{\text{tree}}(\ell_{l}^{\Gamma}) = \sum_{\substack{\Gamma' \geq \Gamma, \\ i \in M_{\Gamma'} \cup S_{\Gamma'}}} \frac{c_{\Gamma', i} m_{\Gamma', i}(\ell_{l}^{\Gamma})}{\prod_{j \in (P_{\Gamma'} \setminus P_{\Gamma})} \rho_{j}(\ell_{l}^{\Gamma})},$$
(3)

which we call the *cut equations*. The set T_{Γ} labels all tree amplitudes corresponding to the vertices in the diagram Γ . The state sum runs over all possible internal states, here the $(D_s - 2)$ gluon helicity states for each internal line of Γ . The right-hand side of the cut equations is expressed in terms of surface terms and master integrands, so that solving the equations directly yields the coefficients of master integrals and no further integral reduction is needed.

If a topology has repeated propagators, any pinch that reduces the multiplicity of the repeated propagator corresponds to a subleading pole in the associated factorization limit. For instance, the fourth topology in the second row of fig. 1 is a subleading pole in the factorization limit associated with the third topology in the first row. As explained in [11], the cut equations (3) directly apply only to the subset of diagrams for which the factorization limit has no subleading pole, but it is nevertheless possible to organize the set of cut equations to compute all coefficient functions $c_{\Gamma,i}$.

With this approach, one can solve the minimal necessary subset of all cut equations which are required to obtain the coefficients of all master integrals. As such, we can omit cut equations of, for example, tadpole and massless bubble diagrams in gluonic amplitudes. This variant of the unitarity approach for computing multi-loop amplitudes is suitable both for analytic and numerical calculations. In what follows, we will focus on its numerical implementation.

Construction of integrand parameterization. For the construction of the integrand (1) we extend the method of ref. [9] to massless propagators and external momenta. The ansatz (1) relies on a suitable set of integration-by-parts (IBP) relations,

$$0 = \int \prod_{l=1,2} d^D \ell_l \frac{\partial}{\partial \ell_j^{\nu}} \left[\frac{u_j^{\nu}}{\prod_{k \in P_{\Gamma}} \rho_k} \right], \qquad (4)$$

which we use to construct the numerators $m_{\Gamma,i}(\ell_l)$. In order to control propagator powers to match the ones of the integrand (1), we construct IBP relations from constrained vector fields [13] which solve,

$$u_i^{\nu} \frac{\partial}{\partial \ell_i^{\nu}} \rho_j = f_j \rho_j, \tag{5}$$

where no summation over the index j is implied. Solutions $\{u_i^{\nu}\}$ of eq. (5) are referred to as IBP-generating vectors. Alternatively, reduction programs [14] can be used to obtain appropriate IBP relations.



FIG. 2: Displayed are the conventions for assigning propagators in a two-loop diagrams.

An important tool for solving eq. (5) and analyzing IBP relations are the natural coordinates [9, 15, 16],

$$\ell_l = \sum_{j \in B_l^p} v_l^j r^{lj} + \sum_{j \in B_l^i} v_l^j \alpha^{lj} + \sum_{i \in B^{ct}} n^i \alpha^{li} + \sum_{i \in B^{\epsilon}} n^i \mu_l^i,$$
(6)

$$r^{li} = -\frac{1}{2} (\rho_{li} - (q_{li})^2 - \rho_{l(i-1)} + (q_{l(i-1)})^2), \qquad (7)$$

which parameterize the strand momenta ℓ_l (l = 1, 2, 3, 3)see fig. 2) in terms of inverse propagators ρ_{li} , and auxiliary variables α^{li} and μ_l^i . The vectors q_{li} are fixed by momentum conservation after imposing $q_{10} = q_{20} = 0$. The vectors n^i form an orthonormal basis transverse to the scattering plane, i.e $n^i \cdot p_j = 0$. Labels in B^{ϵ} refer to directions beyond four dimensions and labels in B^{ct} denote transverse directions within four dimensions. Within the scattering plane, we set up distinct basis vectors v_i^i for each strand of the diagram; the vectors p_i with $i \in B_l^p$ which exit the strand l are completed with additional physical momenta p_i with $i \in B_i^t$, so as to span the whole scattering plane. The vectors v_l^i are dual to the $p_j, v_l^i = (G_l)^{ij} p_j$, with $(G_l)^{ij}$ the inverse of the Gram matrix $(G_l)_{ij} = p_i \cdot p_j$. The new coordinates α^{li}, μ_l^i and ρ_{li} are not independent: momentum conservation $\ell_1 + \ell_2 + \ell_3 + p_b = 0$ removes redundant α_{li} and μ_3^i variables. We often label ρ variables and independent α variables by a single subscript referring to the pair of strand index l and label i. Furthermore, we have the constraint

$$\mu_{ll} \equiv (\mu_l)^2 = \rho_{l0} - \sum_{\nu=0}^3 \ell_l^{\nu} \ell_{l\nu}$$
(8)

for the extra-dimensional momentum squares.

In these coordinates, IBP-generating vectors are [9]

$$u = f_i \rho_i \frac{\partial}{\partial \rho_i} + u_j \frac{\partial}{\partial \alpha^j} + \sum_{l,l'=1,2} f_{l'}^l \mu_l^k \frac{\partial}{\partial \mu_{l'}^k}, \qquad (9)$$

where we denote basis vectors along coordinate lines by the respective partial derivatives. Repeated indices are summed over. We impose rotation symmetry in the extra-dimensional components as manifest in the integrand (1). The vectors must be polynomial when written in canonical coordinates of ℓ_l , requiring first that the coordinate functions f_i , $f_l^{l'}$ and u_i to be polynomial in α^i and ρ_i , and second that the vectors are compatible with the relations in eq. (8). After redundant variables have been eliminated, the compatibility conditions are quadratic in α^i and ρ_i , and read

$$\bar{u}(\mu_{11}) = 2\mu_{11}f_1^1 + 2\mu_{12}f_1^2,$$

$$\bar{u}(\mu_{22}) = 2\mu_{22}f_2^2 + 2\mu_{12}f_2^1,$$

$$\bar{u}(\mu_{12}) = \mu_{12}(f_1^1 + f_2^2) + \mu_{11}f_2^1 + \mu_{22}f_1^2.$$
(10)

We use \bar{u} to denote the μ -independent directions of u in eq. (9) and $\mu_{12} \equiv (\mu_{33} - \mu_{11} - \mu_{22})/2$. The generating set of solutions for the unknowns $f_i, f_{l'}^l$ and u_j are obtained using SINGULAR [17] which we use in addition to universal vectors [9]. We consider the solutions that do not vanish on-shell and keep a generating set of these. An automated implementation of the on-shell variant of the above equations is also available [18].

The simplest IBP-relations are obtained from diagonal rotations [9]. The respective relations are generalizations of the one-loop numerators [5, 6] being traceless completions of the transverse monomials. They can be systematically constructed from traceless completions

$$\begin{aligned} \alpha^{lj} \alpha^{l'j} - b_1 \frac{\mu_{ll'}}{\epsilon}, \quad l, l' \in \{1, 2\}, \\ (\alpha^{lj})^2 (\alpha^{l'j})^2 - b_1 \frac{\mu_{ll}}{\epsilon} (\alpha^{l'j})^2 - b_2 \frac{\mu_{ll'}}{\epsilon} \alpha^{lj} \alpha^{l'j}, \ l \neq l', \end{aligned}$$
(11)

with $j \in B^{ct}$. After multiplying with additional α 's either from B_l^t , $B_{l'}^t$ or B^{ct} the rational constants b_1 and b_2 are fixed to yield expressions that are transverse to the Lorentz structures after loop integration. Monomials with odd powers of α 's from B^{ct} integrate to zero and can be used for numerators as they are. The completion of the IBP relations is obtained by multiplying the IBP-generating vectors with the independent α variables. The numerators are,

$$m_{\Gamma,u}(\ell_l) = \left[-(\nu_i - 1)f_i + \rho_i \frac{\partial f_i}{\partial \rho_i} + \frac{\partial u_j}{\partial \alpha^j} + \left(D - \frac{n_\alpha + 1}{2} \right) (f_1^1 + f_2^2) \right], \quad (12)$$

taking into account the Jacobian factor from eq. (4), see e.g. [19]. In eq. (12), n_{α} denotes the number of independent α_i -variables and ν_i the propagator power.

The numerator decomposition into surface terms and master integrands must be non redundant and complete. The spanning set of IBP-relations is obtained modulo inverse propagators, which allows to check the linear independence with on-shell conditions $\rho_i = 0$ imposed. Finally, the numerators of master integrands are given by the span of irreducible numerators modulo surface terms. In natural coordinates, the irreducible numerators are the monomials in α^i consistent with power counting. It is sufficient to compare the span of IBP-relations and irreducible numerators on a given phase-space point with on-shell conditions imposed to determine a decomposition in terms of master integrals as in eq. (2) [9, 16].

Numerical implementation. We first decompose the amplitude into master integrals and surface terms as in eq. (1) with the method described above. We find two master integrals associated with the first diagram in the first line of fig. 1 (the *double-box*) and one master integral associated with each of the first two diagrams of the third line, the first two diagrams of the fourth line, and the diagram in the last line. For the double-box diagram we choose the scalar and the (irreducible) numerator insertion, and for all other diagrams we choose the scalar integrals.

The coefficients $c_{\Gamma,i}$ in eq. (3) must now be fixed. They are determined numerically by sampling of the on-shell phase spaces ℓ_l^{Γ} , for all $\Gamma \in \Delta'$ [11]. This was implemented in a C++ library, for which the required analytic information - color decomposition (see ref. [20]), hierarchy of cut equations organized to handle subleading poles and IBP relations - is produced in MATHEMATICA. For the four-dimensional spinor algebra we have used tools from the BLACKHAT library [8].

We built an (over)constraining system of linear equations for $c_{\Gamma,i}$ by computing the subtracted product of trees (through off-shell recursions [21]) at randomly sampled phase-space points. Though analytically *D*dimensional, phase-space samples can be constructed with 6-dimensional momenta due to the rotational invariance beyond the 4-dimensional physical slice. The on-shell phase spaces are generated by nested one-loop parameterizations [6, 8]. We single out one of the loops and construct loop momenta on its on-shell phase space. We then input these momenta into the second loop to find two-loop on-shell configurations.

In order to numerically solve the linear systems we constructed for the $c_{\Gamma,i}$, we employ standard linear algebra techniques as implemented in the LAPACK library [22] which uses the BLAS routines [23]. For higher-precision arithmetics, we also use the associated routines from the MPACK libraries [24]. For every $n \times n$ system of equations Mc = a we employ a *PLU* factorization of the square matrix M, in which L is a lower-triangular matrix, U is an upper-triangular matrix and P is a permutation matrix. For over constrained systems of equations, we employ a *QR* factorization (Q a rectangular orthogonal matrix, and R a squared upper-triangular one) for minimizing ||Mc - a||. These factorizations allow for efficient and numerically stable solutions to the systems of equations.

By solving these systems, we numerically determine the coefficients of master integrals for fixed values of Dand D_s . The D_s dependence of master-integral coefficients is at most quadratic and can be reconstructed [7] by evaluating the coefficients with state sums (3) for three different values of $D_s \geq D$. Specifically we use the values $D_s = 6, 7, 8$. The *D* dependence of the coefficients is rational and originates from the D-dependent IBP relations, see eqs. (11) and (12). A priori, the polynomial degrees of the numerator and denominator of the rational function are unknown. However, as this is phase-space independent, it can be determined once and for all in a dedicated run using rational reconstruction techniques in high precision [10, 25]. Further, because the coefficients of the denominators are rational numbers, they can be exactly reconstructed using continued fractions. In this way, after a warm-up phase, one needs only reconstruct a polynomial dependence of known rank.

Finally, to obtain values for the amplitudes (2) we combine the integral coefficients with our own implementation of the loop integrals [26] using the function library of ref. [27]. By setting $D_s = D = 4 - 2\epsilon$ in the coefficients and expanding around $\epsilon = 0$, we recover the value of the bare amplitude as a Laurent series in ϵ in the HV [28] variant of dimensional regularization.

Validation of results. We have computed the two independent helicity configurations with non-vanishing tree amplitudes in the leading- N_c color limit, omitting contributions from closed fermion loops. We normalize the results to the respective tree-level amplitudes \mathcal{A}_0 . We provide numerical values for the coefficients of the Laurent series in ϵ in the HV scheme. For the point $p_{1,3} = -1/2 (1,0,0,\pm 1), p_{2,4} = 1/2 (1,0,\pm\sqrt{3}/2,\pm 1/2),$ we find the following values for the bare amplitudes $(g_s = 1 \text{ and } \mu = 1)$:

$\mathcal{A}/(\mathcal{A}_0 N_c^2)(4\pi)^4$	ϵ^{-4}	ϵ^{-3}	ϵ^{-2}	ϵ^{-1}	ϵ^0
$(1_g^-, 2_g^+, 3_g^-, 4_g^+)$	8.00000	55.6527	176.009	332.296	486.502
$(1_g^-, 2_g^-, 3_g^+, 4_g^+)$	8.00000	55.6527	164.642	222.327	-8.39044

We have checked that the above results agree with the expected universal infrared-pole structure [29], and that they match the results obtained from the analytic expressions of ref. [2]. These comparisons validate the C++ implementation of our numerical unitarity algorithm.

In fig. 3, we show the stability of our calculation by looking at minus the base 10 logarithm of the relative error for the numerical calculation with respect to the analytic result. This is done over 10,000 phase-space points evenly distributed, with a minimum p_T cut on the finalstate partons set to 1/100 the total energy in the centerof-mass frame. The numerical computation has employed single-double precision operations, except when extracting the maximal numerators for which we choose to use double-double precision arithmetics. We have also introduced a rescue system, based on comparisons to the



FIG. 3: Distribution of minus the base 10 logarithm of the relative error for the numerical calculation with respect to the analytic result, over 10,000 phase-space points. The distribution corresponds to the finite $\mathcal{O}(\epsilon^0)$ contribution. The left plot is for the $(1_g^-, 2_g^+, 3_g^-, 4_g^+)$ helicity configuration, and the right plot for $(1_g^-, 2_g^-, 3_g^+, 4_g^+)$.

known pole structure of the amplitude [29], and when failing we recompute the full amplitude in higher floatingpoint precision. We observe that our calculation is precise to better than a per mill relative error for the bulk of phase space and that the rescue system works properly by shifting the left tail of the distribution 16 digits towards the right. When computing with single-double precision over phase space and after reconstruction of the dimensional regulators, our results for master integral coefficients are commonly accurate to 8 digits.

Finally, we have produced results with quadrupledouble precision [30], which gives enough numerical precision to fully reconstruct the analytic form of the amplitudes from the purely numerical computations. This is achieved with the same techniques as for the regulator reconstruction since, after rescaling, the integral coefficients are a function of a single variable.

Conclusions. We have presented a method based on generalized unitarity for automated analytic and numerical computations of two-loop scattering amplitudes in QCD. We have validated our algorithm by comparing numerical results for the leading-color purely-gluonic two-loop four-gluon amplitudes to their known analytic expressions The method is numerically stable and refinements can improve this further in the future. Furthermore, our method can be used to extract the analytic expressions for the amplitude from the purely numerical results. In the last decade, similar developments at one-loop level have led to important predictions for high-multiplicity processes at hadron colliders (see for example Refs. [31]). We are thus optimistic that our approach will be instrumental in yielding new two-loop matrix elements necessary for QCD phenomenology in the near future.

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