Updates to the One-loop Provider NLOX

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Abstract

In this release note we describe the 1.2 update to NLOX, a computer program for calculations in high-energy particle physics. New features since the 1.0 release and other changes are described, along with usage documentation.
I. INTRODUCTION

NLOX is a one-loop provider that allows for the automated calculation of one-loop QCD and electroweak (EW) corrections to Standard Model (SM) scattering amplitudes. Based on Feynman-diagram techniques, it has been developed to optimize the manipulation of symbolic and tensor structures recurring in one-loop amplitudes. The first release of the code (v1.0) \cite{1} consisted of the main tensor-integral reduction library, TRed, and several pre-generated processes. Further processes have been produced upon demand for various projects. All core functionalities of NLOX v1.0 have been presented in detail in Ref. \cite{1} to which we refer.

Since v1.0 the code has seen a substantial number of important additions aimed at improving the numerical stability of the one-loop amplitudes and the interface to external codes. Among the most important additions are improved stability checks in the tensor reduction performed by TRed and new routines that check at runtime the IR pole structure of virtual amplitudes against the IR pole structure of the corresponding real emission, order by order in the QCD+EW couplings. These new IR checks are implemented using color-correlated amplitudes that are now also independently obtainable from the code. Given the impact that these improvements will have on the successful use of the code, we have included them in the new NLOX v1.2 that is being released.

In the following, Sections II and III present a more technical description of all the code’s new features and improvements, while future developments are outlined in Section IV.

II. NEW FEATURES

A. New modes for perturbative expansions

NLOX now has interface support for automatic compilation of all sub-amplitudes that contribute to the same overall power of $\alpha_s$ (QCD) and $\alpha_e$ (QED) in the interference between tree level and tree level or one-loop amplitudes for any given sub-process. This $\alpha$-mode complement the existing possibility of compiling sub-amplitudes by specifying the $g$ ($g^2 = 4\pi\alpha_s$) and $e$ ($e^2 = 4\pi\alpha_e$) power of the interfering tree level and tree level or one-loop amplitudes \cite{1}.

The compiled result with a fixed power of both $\alpha_s$ and $\alpha_e$ can be accessed via the OLP
function `NLOX_OLP_EvalSubProcess` by passing the corresponding string (`cp`) specifying the coupling-power combination. In a C++ program this OLP function takes the form:

```
NLOX_OLP_EvalSubProcess(isub, type, cp, p, next, mu, rval, acc)
```

where the arguments follow the BLHA standard [2]:

- **isub**: Integer number specifying the index of the desired sub-process as defined in the sub-process list in `nlox_process.h`.
- **type**: Character string specifying the interference type, both `tree_tree` and `tree_loop` are supported.
- **cp**: Character string specifying the coupling-power combination of the interference type in question, both `$g_{i}^{'e_{j}'}g_{i}^{'j}e_{j}$` and `$a_{X}e_{Y}$` (where $X = (i' + i)/2$ and $Y = (j' + j)/2$) are supported.
- **p**: Array of double-precision numbers specifying the external momenta and masses, each momenta must be followed by its mass.
- **next**: Integer number specifying the number of external particles.
- **mu**: Double-precision number specifying the renormalization scale (in GeV).
- **rval**: Return value pointer, the container must allow for 3 double-precision numbers to be stored corresponding to double pole, single pole, and finite part.
- **acc**: Accuracy pointer, the container must allow for a single double-precision value to be stored.

In a Fortran program this OLP function takes extra arguments specifying the length of the interference type and of the coupling power combination:

```
NLOX_OLP_EvalSubProcess(isub, type, ltyp, cp, lcp, p, next, mu, rval, acc)
```

where the extra arguments of this function are:

- **ltyp**: Integer specifying the length of the interference type string.
- **lcp**: Integer specifying the length of the coupling-power combination string.
A detail worth mentioning regarding the usage of the two different specifications for coupling powers in NLOX is the following. In the $\alpha$-mode, where the character string \( cp \) is in the form $a\!sXaeY$, all sub-amplitudes with the same overall power of $\alpha_s$ and $\alpha_e$ are summed over automatically. In contrast to that, when the character string \( cp \) is specified in the form $g'i'egiej$, the various sub-amplitudes contributing to the same overall power of $\alpha_s$ and $\alpha_e$ can be accessed individually, but must then be summed up manually.

B. Color-correlated output

NLOX is now capable of providing color-correlated Born-level matrix elements $B_{ij}$. The normalization convention used is:

$$B_{ij} = \langle M^{C_1,\ldots,C_i,\ldots,C_j,\ldots,C_m} | (T^a)_{C_iD_i} (T^a)_{C_jD_j} | M^{C_1,\ldots,D_i,\ldots,D_j,\ldots,C_m} \rangle$$

where the matrices $T^a$ denote the generators of the $SU(3)$ algebra and the indices $\{C_i, D_i\}$ are generic indices associated to the $SU(3)$ representation under which the $i$-th particle transforms. More specifically [3] the $(T^a)_{C_iD_i} \equiv T_i$ are defined as:

$$
(T^a)_{C_iD_i} = \begin{cases} 
(t^a)_{\alpha\beta} & \text{for initial quarks and final anti-quarks}, \\
-(t^a)_{\beta\alpha} & \text{for initial anti-quarks and final quarks}, \\
(t^a)_{cb} = if^{cab} & \text{for gluons},
\end{cases}
$$

where $(t^a)_{\alpha\beta}$ ($\alpha, \beta = 1, 2, 3$) and $(T^a)_{cb} = if^{abc}$ ($a, b, c = 1, \ldots, 8$) are the color-charge matrices in the fundamental and adjoint representation respectively, $f^{abc}$ are the $SU(3)$ structure constants, and $(T_i)^2 = C_i$ with $C_i = C_A = N$ if $i$ is a gluon and $C_i = (N^2 - 1)/2N$ if $i$ is a quark or an antiquark ($N = 3$ for $SU(3)$).

For direct evaluation, there is a dedicated OLP level function that calls for the evaluation of color-correlated matrix elements:

```
NLOX_OLP_EvalSubProcess_CC(isub, type, cp, p, next, mu, borncc, acc)
```

which can only be called for Born-level matrix elements. The container that \texttt{borncc} points to must be able to store the uncorrelated Born-level matrix element as well as the
components for which \( j > i \), while the components with \( i > j \) can be obtained via symmetry from the \( B_{ij} \). The first element in the container is reserved for the uncorrelated Born, and the subsequent \([n(n-1)]/2\) elements correspond to the components of \( B_{ij} \) using lexicographical order on \((i,j)\).

For Fortran programs the OLP function takes extra arguments specifying the length of the interference type as well as the coupling power combination:

\[
\text{NLOX\_OLP\_EvalSubProcess\_CC}(\text{ish}, \text{type}, \text{ltyp}, \text{cp}, \text{lcp}, \text{p}, \text{next}, \text{mu}, \text{rval}, \text{acc})
\]

where the extra arguments of this function are:

- \text{ltyp}: Integer specifying the length of the interference type string.
- \text{lcp}: Integer specifying the length of the coupling-power combination string.

C. Runtime amplitude-level pole checks

Routines that calculate the IR pole structure of the real emission associated to a given Born amplitude have been newly implemented within NLOX, but are only computed in the \(\alpha\)-mode of coupling-power specification. The virtual IR poles are computed independently in the combination of loop and counterterm diagrams, and must cancel the real IR poles in the \(G_\mu\) input scheme.\(^1\) If real and virtual IR poles must cancel against each other, checking for the goodness of zero of their sum can be used to provide a check on the stability of the tensor reduction algorithm. The user has access to this new feature via the \text{acc} flag of the \text{NLOX\_OLP\_EvalSubProcess} function. This flag has different behavior depending on the particular type of \text{cp} the user specifies:

- \text{cp=gij'g'ej}: \text{acc} is either 0 for success or \(-1\) for failure, where failure is internally determined by \text{TRed} as described in \(\text{III.A}\).

\(^1\) Because NLOX only allows nonzero masses for the \(b\) and \(t\) quarks, EW renormalization in the \(\alpha(0)\) scheme formally produces IR poles arising from massless fermions that remain after combination with those arising from real radiation, and must be compensated externally. Thus, in the \(\alpha(0)\) scheme, the IR pole-checking feature is only useful for strictly QCD corrections, while it works for both QCD and EW corrections in the \(G_\mu\) scheme (\text{GmuScheme = true}).
• **cp=asXaeY**: acc is $-1$ for a TRed failure. In case of a TRed success the acc flag returns the accuracy of the virtual IR single pole relative to the real IR single pole.

The calculation of the real IR poles is based on the dipole-subtraction formalism and it requires the internal evaluation of color-correlated Born matrix elements $^3$.

**D. Runtime parameter setting**

In order to change physical parameters at runtime, NLOX now supports the Les Houches $^2$ standard function `OLP_SetParameter()`:

```
NLOX_OLP_SetParameter(para, re, im, ierr)
```

whose arguments are:

- **para**: Character array, the name of the parameter to be changed. The currently supported names are:
  - "**alpha_e**": $\alpha_e$, the QED fine structure constant.
  - "**alpha_s**": $\alpha_s$, the QCD coupling constant.
  - "**mb**, "**mt**, "**mH**, "**mW**, "**mZ**": masses of supported massive particles.
  - "**wH**, "**wW**, "**wZ**": widths of supported particles. At present unstable fermions are not officially supported, and giving a nonzero width to an external particle will result in undetermined behavior.
  - "**nlf**" the number of light quark flavors to be used for renormalization purposes (see Appendix A.3 of Ref. $^1$ for more details).
  - "**nhf**" the number of heavy quark flavors to be used for renormalization purposes (see Appendix A.3 of Ref. $^1$ for more details).
  - "**mu**" the renormalization scale.

It is recommended that one change these values only as often as necessary. For masses and widths in particular, changing the value can result in expensive reallocations and computations.
• **re**: Pointer to a double precision number holding the new real part of the value to be set.

• **im**: Pointer to a double precision number. This should be a dummy variable, as NLOX does not currently support setting parameters to complex values through this function.

• **ierr**: Pointer to an integer to store the return flag of the function. Set to 1 if successful and 2 if the name is unknown.

For Fortran programs the `SetParameter` function takes an extra argument:

```
NLOX_OLP_SetParameter(para, lpara, re, im, ierr)
```

where the extra argument of this function is:

• **lpara**: Integer specifying the length of the parameter name string.

Derived complex parameters arising in the complex mass scheme [4], if selected, are calculated using the complex masses, which are built from real masses and widths and recomputed when one is set.

### III. IMPROVEMENTS AND OTHER CHANGES

#### A. TRed stability checks

Since its original release, the TRed library has internally checked the stability of the tensor-integral reduction. Its primary check is to compare the single pole term (the coefficient $c_1$ in the expansion $c_2 \epsilon^{-2} + c_1 \epsilon^{-1} + c_0$ of a given tensor-integral coefficient) to an internal fast-evaluating library for coefficients that are infrared finite. This is a direct cross-check, that allows early correction of individual coefficients through recalculation at higher precision, and acts as a first-pass filter of potential instabilities, and has now been complemented by the IR-pole check described in Section II C. In this new release of NLOX we have improved its effectiveness as described in the following.

The driver of instability for the primary reduction method, Passarino-Veltman [5], is unstable matrix inversion involving the Gram matrix $G_{ij} \equiv 2p_i \cdot p_j$ for loop internal momenta.
In particular, the determinant of this matrix becomes small as it becomes degenerate, and
as it appears explicitly in the denominator of reduction formulae, an imprecise cancellation
in the numerator of the reduction can result in large incorrect results. To guard against
this problem, in previous versions TRed has compared the size of the Gram determinant
to an appropriate-scaling quantity, $E^{2(N-1)}$ for $E$ a scale in the problem. However, one
can improve on the sensitivity and specificity of this test with more information, reducing
the failures for acceptable phase space points and catching others that may have been
problematic. To this end, we have improved the test to more directly check the instability
of the linear system.

A geometric interpretation of a determinant is that it is the volume of the parallelepiped
spanned by the matrix’s row (or column) vectors. As the vectors become linearly dependent,
the volume of this space shrinks to zero, and the space spanned by them loses a dimension.
Therefore, a direct measure of the smallness of the determinant compares it to the maximal
volume such a space would have with the same-sized vectors, i.e., if they were orthogonal.
Our new test compares $\det G_{ij}$ to $\prod_i |\vec{G}_i|$ (where $\vec{G}_i$ denotes the array of the $G_{ij}$ for fixed $i$).
The specificity of this test has allowed us to pass many configurations that would previously
have been thrown out, even while preventing unhandled instabilities that could occur in
collinear configurations for some processes.

Since TRed relies on external scalar integral libraries for the endpoint of its reduction, it
is only as good as the precision of those libraries. In particular, in the small determinant
case above, combinations of scalar integrals appearing may cancel in the limit of degenerate
configurations. While TRed will attempt to do the reduction in higher precision, if the scalars
only match to a lower precision, this can result in poor behavior regardless. Therefore
we have reconfigured the installation of the default scalar library, OneLOop [6], to install
quadruple-precision versions of its functions, and adjusted TRed to make use of them as
appropriate.

B. Code size optimizations

Expressions resulting from the algebraic construction of the expression for a process
squared amplitude naturally can be large for complicated processes, especially if many
masses are involved or the theory has non-trivial expressions for interactions, as in the
case of the broken electroweak theory. We have focused on simplifying expressions, especially finding overall factors, and finding common structures such that the resulting code size is smaller. These optimizations can result in a reduction of code size of as much as a factor of two in extreme situations compared to the version 1.0 release. These optimizations improve runtime speed as well if the speed is process-cache or memory-speed limited.

Since much of the resulting algebraic data has been removed from code generation entirely, and placed into process data files, this is the dominant contribution to a process package size. We have eliminated some empty files and redundant structures to further reduce the size of a process package.

IV. OUTLOOK

We have described the important changes to NLOX since its original release. The main focus has been on numerical stability. We have reorganized internal integral stability checks for accuracy and efficiency. We have also added a new stability check by implementing the IR singular part of the real radiation using the dipole-subtraction formalism, and exploiting the finiteness of the combined real and virtual contribution after the respective IR poles cancels at the level of the final answer.

The implementation of IR-pole checks based on the dipole formalism has also exposed a new functionality to the user, that of Born-level color-correlated amplitudes, which may be of use to users wishing to interface NLOX to Monte Carlo simulators requesting these amplitudes.

This release has also seen the implementation of runtime parameter setting, further implementing the Les Houches Accord next-to-lowest-order function interface and making the process of interfacing NLOX to external programs more convenient.

While this 1.2 release and its predecessor, 1.1, have focused on stability and ease of use, we anticipate the next releases will focus on speed and size efficiency, while also continuing to improve the ease of use and organization of the non-public process archive generation features so that the full package may be released.

To access the host URL for the NLOX package, please go to http://www.hep.fsu.edu/~nlox.
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[1] S. Honeywell, S. Quackenbush, L. Reina, and C. Reuschle, Comput. Phys. Commun. 257, 107284 (2020), 1812.11925.
[2] S. Alioli et al., Comput. Phys. Commun. 185, 560 (2014), 1308.3462.
[3] S. Catani and M. H. Seymour, Nucl. Phys. B485, 291 (1997), [Erratum: Nucl. Phys. B510,503(1998)], hep-ph/9605323.
[4] A. Denner, S. Dittmaier, M. Roth, and L. H. Wieders, Nucl. Phys. B724, 247 (2005), [Erratum: Nucl. Phys.B854,504(2012)], hep-ph/0505042.
[5] G. Passarino and M. J. G. Veltman, Nucl. Phys. B160, 151 (1979).
[6] A. van Hameren, Comput.Phys.Commun. 182, 2427 (2011), 1007.4716.