

FormTracer

A Mathematica Tracing Package Using FORM

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Abstract

We present *FormTracer*, a high-performance, general purpose, easy-to-use Mathematica tracing package which uses FORM. It supports arbitrary space and spinor dimensions as well as an arbitrary number of simple compact Lie groups. While keeping the usability of the Mathematica interface, it relies on the efficiency of FORM. An additional performance gain is achieved by a decomposition algorithm that avoids redundant traces in the product tensors spaces. *FormTracer* supports a wide range of syntaxes which endows it with a high flexibility. Mathematica notebooks that automatically install the package and guide the user through performing standard traces in space-time, spinor and gauge-group spaces are provided.

Keywords: Trace, FORM, Mathematica, Feynman diagrams

PROGRAM SUMMARY

Program Title: FormTracer

Licensing provisions: GPLv3

Programming language: Mathematica and FORM

Computer: any computer running FORM 4.1 and Mathematica 10 or higher

Nature of problem: efficiently compute traces of large expressions

Solution method:

The expression to be traced is decomposed into its subspaces by a recursive Mathematica expansion algorithm. The result is subsequently translated to a FORM

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script that takes the traces. After FORM is executed, the final result is either imported into Mathematica or exported as optimized C/C++/Fortran code.

Unusual features:

The outstanding features of *FormTracer* are the simple interface, the capability to efficiently handle an arbitrary number of Lie groups in addition to Dirac and Lorentz tensors, and a customizable input-syntax.

1. Introduction

Computer-algebraic tools are the backbone of many recent advances in theoretical high energy physics. This is particularly true in perturbation theory, where a large variety of tools for different stages of these very demanding calculations is available, see [1–3] for reviews. But also recent advances in the application of non-perturbative continuum functional methods, see [4–14] for reviews, require the ability to perform traces over increasingly complicated algebraic expressions. These stem mainly from the need to evaluate the one- and two-loop diagrams of these methods at off-shell momenta as well as expressing the appearing products of dressed propagators and vertices in terms of ever larger bases of tensors structures, see e.g. [15–23]. To summarize, typical workflows in perturbative as well as non-perturbative calculations involve the evaluation of traces in different subspaces, ranging from Lorentz and Dirac to group traces.

Here, we present *FormTracer*, a dedicated tracing tool that uses FORM [24, 25] in connection with an efficient expansion algorithm in Mathematica. Applying *FormTracer* requires only basic Mathematica skills, since all its features can be accessed directly from the Mathematica interface. The translation into FORM scripts is completely automated and consequently no knowledge of FORM syntax is required. The final results are either imported into Mathematica for further manipulations or exported as optimized C/C++/Fortran code with FORM’s optimization routine [26]. Furthermore, many examples and an automatic installation routine are provided in Mathematica notebooks that include all the necessary information for performing traces in standard applications.

Crucial parts of *FormTracer* have been developed during the course of [19, 20]. By now, *FormTracer* represents an integral part of the workflow within the fQCD collaboration [27] and has been used during the derivation of the equations in [20, 23, 28–30].

Since most of the information needed for applying *FormTracer* is contained already in the Mathematica notebooks referred in Sec. 2, the remainder of this paper focuses on providing additional theoretical background. In particular, we give a list of features in Sec. 3 and summarize relevant properties of simple compact Lie groups in Sec. 4. The treatment of the fifth gamma matrix in general dimensions as well as finite temperature and density applications are discussed in Sec. 5. We compare *FormTracer* to similar tools in Sec. 6 and explain the decomposition algorithm in Sec. 7. We discuss further algorithmic details in Sec. 8 before we conclude in Sec. 9.

2. Installation and Usage

2.1. Installation and Quickstart Guide

FormTracer requires FORM¹ version 4.1 and Mathematica 10.0 or higher. We recommend to install *FormTracer* with the fully automated installation script, which can be downloaded and started by evaluating

```
In[1]:= Import["https://raw.githubusercontent.com/FormTracer/\
FormTracer/master/src/FormTracerInstaller.m"]
```

in a Mathematica input cell. If FORM is not already installed on your computer, it can be installed automatically during the installation process. As an alternative to the automatic installation, one can also download *FormTracer* manually from [33] and install it by copying it into Mathematica's application folder. Three notebooks with examples are available for download:

- <https://raw.githubusercontent.com/FormTracer/FormTracer/master/src/Examples/FormTracerShowcase.nb>
- <https://raw.githubusercontent.com/FormTracer/FormTracer/master/src/Examples/FormTracerMinimalExample.nb>
- <https://raw.githubusercontent.com/FormTracer/FormTracer/master/src/Examples/FourQuarkInteraction.nb>

¹ FORM is licensed under the GPLv3. The source code can be obtained from [31] and readily compiled executables are available at [32].

The first notebook provides an extensive overview over the features of *FormTracer* based on many example traces, whereas the second provides the minimal prerequisite for being able to perform simple traces over space-time, spinor and gauge group indices. To demonstrate *FormTracer*'s performance, we provide a third notebook with a more complicated example, namely the tracing of four-quark interaction diagrams performed in [20]. All examples can also be found in the examples folder in the installation directory. The first two examples provide an input cell to execute the automatic installation script as shown above. While these example files should be understood as quickstart guides to start using *FormTracer* as fast as possible, we also provide an extensive documentation in Mathematica's Documentation Center. A good overview is given on the main page that can be accessed by simply searching for *FormTracer* in the Documentation Center.

2.2. Basic Usage Examples

Once installed, *FormTracer* is loaded via

```
In[2]:= Needs["FormTracer`"]
```

FormTracer requires to define a custom notation which makes it easily adaptable to the output of external diagram generators. Below, we define our notation for Lorentz tensors and group tensors for two $SU(N)$ groups. For more information on the individual functions, see the respective help pages in Mathematica's Documentation Center.

```
In[3]:= DefineLorentzTensors[deltaLorentz[mu, nu], vec[p, mu], sp[p, q],
    eps[], deltaDirac[i, j], gamma[mu, i, j], gamma5[i, j]];
DefineGroupTensors[{
    {SUNfund, {color, Nc}, deltaAdj[a, b],
    f[a, b, c], deltaFund[i, j], T[a, i, j]},
    {SUNfund, {flavor, Nf}, deltaAdjFlav[a, b], fFlav[a, b, c],
    deltaFundFlav[i, j], TFlav[a, i, j]}}];
DefineExtraVars[alpha, Mpsi, Zpsi, xi, g];
```

FormTracer requires all further external variables to be declared before usage since FORM requires it. In the last line, we defined all variables that are used in the examples below. Now, one can start tracing

```
In[4]:= FormTrace[vec[p, nu] deltaLorentz[mu, nu]
    vec[q, mu] deltaFund[i, j] deltaFund[j, i]]
```

```
Out[4]= Nc sp[p, q]
```

or

```
In[5]:= FormTrace[vec[p,nu]vec[q,rho]gamma[mu, i1,i2]
                gamma[nu,i2,i3]gamma[rho,i3,i4]gamma[mu,i4,i1]]
```

```
Out[5]= 16 sp[p, q]
```

FormTracer supports a shorthand notation for Dirac matrices that allows to leave out auxiliary indices. For example, one can evaluate the above Dirac trace $\text{Tr } \gamma^\mu \not{p} \not{q} \gamma^\mu$ simply via

```
In[6]:= FormTrace[gamma[{mu,vec[p],vec[q],mu}]]
```

```
Out[6]= 16 sp[p, q]
```

As a more complex example from QCD, consider one-loop quark contribution to the gluon propagator that is given by the following uncontracted expression

```
In[7]:= testExpr = deltaAdj[colAdja, colAdjb]*
          (deltaLorentz[Mu, Nu] + xi (vec[p, Mu] vec[p, Nu])/sp[p, p])*
          g*gamma[Mu, i1, i4]*deltaFundFlav[flavFunda, flavFundd]*
          T[colAdja, colFunda, colFundd]*(deltaDirac[i2, i1] Mpsi +
          I gamma[Rho, i2, i1] vec[-p - q, Rho] Zpsi )/
          (Mpsi^2 + sp[p + q, p + q] Zpsi^2)*
          deltaFundFlav[flavFundb, flavFunda]*
          deltaFund[colFundb, colFunda]*g*gamma[Nu, i3, i2]*
          deltaFundFlav[flavFundc, flavFundb]*
          T[colAdjb, colFundc, colFundb]*
          (deltaDirac[i4, i3] Mpsi + I gamma[Sigma, i4, i3]*
          vec[q, Sigma] Zpsi)/(Mpsi^2 + sp[q, q] Zpsi^2)*
          deltaFundFlav[flavFundd, flavFundc]*
          deltaFund[colFundd, colFundc];
```

which yields

```
In[8]:= Simplify[FormTrace[testExpr]]
```

```
Out[8]= (2 g^2 (-1 + Nc^2) Nf (2 xi Zpsi^2 sp[p, q] sp[p, p + q] +
          sp[p, p] (Mpsi^2 (4 + xi) - (2 + xi) Zpsi^2 sp[q, p + q]))) /
          (sp[p, p] (Mpsi^2 + Zpsi^2 sp[q, q]) (Mpsi^2 +
          Zpsi^2 sp[p + q, p + q]))
```

For further usage examples consult the documentation in Mathematica's Documentation Center or one of the example notebooks.

3. Features

Here, we summarize the main features of *FormTracer*:

- evaluation of (Euclidean) Lorentz/Dirac traces in arbitrary dimensions, and traces over an arbitrary number of group product spaces, see Sec. 4
- high performance due to FORM backend combined with an efficient decomposition algorithm in Mathematica, see Sec. 7
- supports
 - the γ_5 matrix in general dimensions within the Larin scheme, see Sec. 5.1
 - a special time-like direction for (Euclidean) finite temperature and density applications, see Sec. 5.2
 - partial traces involving open indices
 - creation of optimized output (including bracketing) using FORM's optimization algorithm [26] for further numerical processing in C/C++/Fortran
 - user-defined combined Lorentz tensors and corresponding identities, e.g. (transverse and longitudinal) projectors and their orthogonality relations, for speedup
- intuitive, easy-to-use and highly customizable Mathematica frontend
- convenient installation and update procedure within Mathematica

4. Simple Compact Lie Groups

FormTracer includes different group tracing algorithms that are implemented in FORM. The most general algorithm is provided by the FORM color package [34] and allows to take traces of arbitrary simple compact Lie groups. Furthermore, we include explicit tracing algorithms for the fundamental representation in $SU(N)$, $SO(N)$ and $Sp(N)$, adapted from routines

published with the color package [34] that use the Cvitanovic algorithm [35] with additional support for partial traces. Finally, we include dedicated tracing algorithms for the fundamental representations in $SU(2)$ and $SU(3)$ that support partial traces, explicit numerical indices as well as transposed group generators. The use of explicit numerical indices requires to work in explicit representations. For $SU(2)$ and $SU(3)$ we choose generators proportional to Pauli and Gell-Mann matrices, respectively. Note that the fundamental $SU(N)$ tracing algorithm also supports partial traces but does not guarantee the same degree of simplification as the specific $SU(2)$ and $SU(3)$ routines. Due to the modular structure of the tracing procedure, the inclusion of further tracing algorithms at a later stage is easily possible.

The definitions of the group constants follow those of the color package [34], which we repeat here for the reader's convenience. We consider simple Lie algebras with (Hermitian) generators T_R , which obey

$$[T_R^a, T_R^b] = i f^{abc} T_R^c, \quad (1)$$

where f^{abc} denote the structure constants. The dimensions of the representation R and the adjoint representation are denoted by N_R and N_A , respectively. Furthermore, we define quadratic Casimir operators C_R and C_A via

$$(T_R^a T_R^a)_{ij} = C_R \delta_{ij} \quad \text{and} \quad f^{acd} f^{bcd} = C_A \delta^{ab}. \quad (2)$$

It only remains to fix the normalization:

$$\text{Tr} T_R^a T_R^b = I_2(R) \delta^{ab}, \quad (3)$$

where $I_2(R)$ denotes the second-order index of the representation R . Note that all tracing algorithms except for the FORM color package produce tracing results just in terms of the dimensions N_R and N_A with all other group constants set to their default values. In the case of $SU(N)$ in the fundamental representation, these values are given by

$$C_R = \frac{N_R^2 - 1}{2N_R}, \quad C_A = N_R, \quad I_2(R) = \frac{1}{2}. \quad (4)$$

5. Dirac and Lorentz Tracing

5.1. Dirac Traces in General Dimensions

Although FORM has built-in support for Dirac Traces in d dimensions it does not come with a built-in solution for the handling of the fifth gamma

matrix, which is defined as an inherently four-dimensional object. Nevertheless, the generalization of the γ_5 matrix to d dimensions is very important, in particular for applications using dimensional regularization. The implementation of the fifth gamma matrix in $d \neq 4$ dimensions represents a subtle procedure and different prescriptions exist. Here, we closely follow [36, 37] and implement support for the fifth gamma matrix by means of the Larin scheme [36] translated to Euclidean space-time, which exploits the relation

$$\gamma_\mu \gamma_5 = \frac{1}{3!} \epsilon_{\mu\nu\rho\sigma} \gamma_\nu \gamma_\rho \gamma_\sigma. \quad (5)$$

For non-trivial expressions containing γ_5 matrices, *FormTracer* applies the following algorithm to every spin line:

1. Replace any occurring $\gamma_5 \gamma_5$ with the unit matrix, $\gamma_5 \gamma_5 \rightarrow 1$.
2. Read each Dirac subtrace such that no γ_5 is found on the leftmost position and replace all γ_5 matrices using Eq. (5).
3. Contract all epsilon tensors that do not stem from step 2.
4. Contract all remaining epsilon tensors.
5. Perform Dirac trace in d dimensions with FORM.

The separate contraction of different sets of epsilon tensors in 3. and 4. is necessary, since there is no Schouten identity for general $d \neq 4$, which guarantees the equivalence of different contraction orders in four dimensions. When only a single γ_5 matrix needs to be traced, a faster procedure based on an implicit application of Eq. (5) can be used [37]. By setting *FastGamma5Trace[True]*, *FormTracer* applies Eq. (5) to all but the last γ_5 matrix, which is then traced with this faster strategy.

Due to the intricacies of the definition of γ_5 in $d \neq 4$ dimensions, we encourage users to ensure that the implemented prescription is suitable for their specific application. Particular caution is necessary in the case of multiple disconnected spin lines in the presence of connecting epsilon tensors.

5.2. Finite Temperature and Density Tracing

FormTracer has a built-in functionality for a special time-like direction that is useful for Euclidean finite temperature and density applications. It supports the definition of space-like vectors

$$p_s = \begin{pmatrix} 0 \\ \vec{p} \end{pmatrix}, \quad (6)$$

which hold the spatial components of the corresponding full vectors

$$p = \begin{pmatrix} p_0 \\ \vec{p} \end{pmatrix}. \quad (7)$$

By definition, these vectors obey the following relations:

$$p \cdot_s q \equiv \vec{p} \cdot \vec{q} = p_s \cdot q_s = p_s \cdot q, \quad (8)$$

where the space-like inner product \cdot_s has been introduced, which is supported by *FormTracer*. In the evaluation of traces, the spatial vectors, p_s , with full dimensions are kept until the trace is performed. The traced expressions are then represented in terms of standard and space-like inner products using Eq. (8). This implementation of finite temperature is limited to Euclidean signature, which is sufficient for finite temperature and density applications in equilibrium.

6. Comparison with Other Programs

FormTracer was designed for the specific task of evaluating Lorentz, Dirac and group traces. Our focus in its development was on usability, performance and the ability to handle very large expressions. In a typical workflow, these expressions are provided by further external programs that generate diagrams. One example for such a tool with particular relevance for calculations in non-perturbative functional methods is DoFun [38]. In perturbative applications, input e.g. from FeynArts [39] or QGRAF [40] as popular Feynman diagram generators is feasible.

There is a large number of tools, which have at least a partial overlap with *FormTracer* in their functionalities, see for example [1–3] for reviews on computer-algebraic methods in perturbative applications. In the following, we provide a comparison to programs that are from our point of view most straightforwardly adaptable to tracing applications in the context of non-perturbative functional method calculations. Although these tools were designed with more general applications in mind, we restrict the following comparison to their tracing capabilities.

- FORM [24–26, 34] is a dedicated tool for high-performance symbolic calculations. It is a standalone program that comes with its own specialized input language. It has a built-in capability of taking Lorentz

and Dirac traces as well as group traces involving arbitrary simple Lie groups using the color package [34]. The primary focus of FORM lies in speed and the ability to handle even very large symbolic expressions. However, the usage of FORM poses a rather steep learning curve for the beginner. *FormTracer* aims to overcome this limitation by combining a Mathematica frontend in combination with a specialized expansion algorithm in Mathematica while still making use of the computational power of FORM in the background. By construction, it is always possible to write native FORM code for a specific tracing application that is as fast as the code generated automatically by *FormTracer*, but the latter is for many applications the more convenient choice.

FormLink [41] provides a way of accessing FORM via Mathematica to execute FORM commands and imports results back into Mathematica. However, it still requires the user to write FORM code and is therefore very close to FORM itself in its usage.

- FeynCalc [42–44] is a popular Mathematica package for the symbolic semi-automatic evaluation of Feynman diagrams and allows in particular to evaluate Dirac and Lorentz traces in arbitrary dimensions as well as fundamental $SU(N)$ group traces. Unlike *FormTracer*, it includes a rich set of tools beyond the ability of taking traces such as tensor reduction algorithms for one-loop integrals that make it particularly suited for perturbative applications. On the other hand, *FormTracer* is a specialized tracing tool and the complexity of expressions it can handle as well as its performance are typically only limited by FORM itself. As a consequence, *FormTracer* is often more than an order of magnitude faster than FeynCalc in examples typically occurring in non-perturbative functional QCD calculations.
- HEPMath [45] is a Mathematica package that extends the functionality of Tracer [46] and provides algorithms for high energy physics computations and therefore includes support for Lorentz, Dirac and $SU(3)$ group traces. In its functionality, HEPMath is similar to FeynCalc, which it aims to surpass in usability and flexibility without focus on performance. It is designed as a convenience tool with a more general scope than *FormTracer* however with a significantly smaller functionality in the tracing capability itself.

Apart from this incomplete selection, we want to acknowledge dedicated

tools for the evaluation of diagrams such as Mincer [47], CompHEP [48], DIANA [49], FormCalc [50], MATAD [51], GRACE [52], SANCscope [53], MadLoop [54], GOSAM [55], Package X [56, 57] and Forcer [58] as well as computer algebra systems/packages for tensor algebra with tracing capabilities like GiNaC [59] GAMMA [60], Cadabra [61], SymPy [62], xAct [63, 64] and Redberry [65].

7. Decomposition of Tensor Classes

This section explains details of the expansion algorithm, which is hidden from the user. Let x be an untraced expression, of which the trace over n Lie groups as well as Dirac and Lorentz space is to be taken. The straightforward way to carry out the trace in x would be to fully expand x into a sum of simple products of tensors and repeatedly apply the appropriate tensor identities to the summands. However, this strategy almost always entails multiple calculations of identical subtraces. Since FORM fully expands all expressions, we decompose x into its subspaces in Mathematica by bringing it into the form

$$x = c_0 \sum_{i_0} C_{i_0} \sum_{i_1} C_{i_0 i_1} \cdots \sum_{i_n} C_{i_0 i_1 \dots i_n} L_{i_0 i_1 \dots i_n}. \quad (9)$$

Here, c_0 represents a scalar prefactor, $C_{i_0 \dots i_j}$ contains only tensors of the j -th group, $L_{i_0 i_1 \dots i_n}$ consists only of Lorentz and Dirac tensors and the summation boundary of i_j in Eq. (9) depends on i_0, \dots, i_{j-1} . In addition to the considerable performance gain due to the uniqueness of the tensors $C_{i_0 \dots i_j}$, this decomposition allows to take the traces of the individual Lie groups separately. For tracing the combined Lorentz and Dirac tensors $L_{i_0 i_1 \dots i_n}$ in Eq. (9), we provide two possibilities. By default, no further manipulation is performed and we let FORM handle the evaluation of the $L_{i_0 i_1 \dots i_n}$'s.

8. Additional Algorithmic Details and Optimization

8.1. Partial Traces over Lorentz Tensors

In some cases, where the scalars $L_{i_0 i_1 \dots i_n}$ in Eq. (9) are very large, a further decomposition can improve the performance by splitting the full trace into

partial intermediate traces. The decomposition can be turned on with the option `DisentangleLorentzStructures[True]`, which first groups the expressions $L_{i_0 i_1 \dots i_n}$ into a sum of Lorentz and Dirac scalars

$$L_{i_0 i_1 \dots i_n} = \sum_j l_{i_0 i_1 \dots i_n; j}. \quad (10)$$

Next, each of these summands is written as,

$$l_{i_0 i_1 \dots i_n; j} = \prod_{f=1}^{N_j} \left(\prod_{g=1}^{N_{jf}} l_{i_0 i_1 \dots i_n; jfg}^{\{\mu_{jfg}\}} \right). \quad (11)$$

Here, the factors of the outer product are the smallest possible Lorentz scalars and the factors of the inner product the smallest possible, already traced, Dirac scalars that allow for such a representation. The superscripts $\{\mu_{jfg}\}$ denote a set of Lorentz indices and the factors are ordered such that

$$\{\mu_{jfg}\} \cap \{\mu_{jfg+1}\} \neq \emptyset. \quad (12)$$

To avoid large expressions by possibly exploiting intermediate simplifications, the Lorentz traces are evaluated successively,

$$\begin{aligned} & \text{Tr} \left(\prod_{g=1}^{N_{jf}} l_{i_0 i_1 \dots i_n; jfg}^{\{\mu_{jfg}\}} \right) \\ &= \text{Tr} \left(l_{i_0 i_1 \dots i_n; jf1}^{\{\mu_{jff1}\}} \text{Tr} \left(\dots \text{Tr} \left(l_{i_0 i_1 \dots i_n; jf(N_{jf}-1)}^{\{\mu_{jff(N_{jf}-1)}\}} l_{i_0 i_1 \dots i_n; jfN_{jf}}^{\{\mu_{jffN_{jf}}\}} \right) \right) \right), \end{aligned} \quad (13)$$

and the results are multiplied and summed only at the very end. This feature has been crucial for quantum gravity applications, in particular for tracing the four-graviton vertex equation [66].

8.2. Other Algorithmic Improvements

We implemented two further improvements that greatly reduce the number of terms in many of our standard applications. Internal loop momenta are in general sums of the loop and external momenta. Simply expanding all vector sums (e.g. $(p+q)_\mu \rightarrow p_\mu + q_\mu$) leads to an unnecessarily large number of terms. Thus, we replace sums of vectors by abbreviations and reinsert the explicit momenta after the tracing process. Although this can

prevent cancellations in the final result, we found these abbreviations to be very advantageous for the performance as well as the size of the final result in the general case involving off-shell momenta.

By default, FORM expands all powers of sums, even if the sums only contain scalars. In this special case, however, an expansion is not necessary to evaluate the traces. Therefore, we prevent FORM from expanding powers over sums of scalars by using a user-defined power function symbol in the FORM code.

9. Conclusion

We presented the dedicated tracing package *FormTracer* for Mathematica. Its most notable features are its usability, performance, and the capability to efficiently handle an arbitrary number of Lie groups as well as Dirac and Lorentz tensors in arbitrary dimensions. This includes an algorithm to deal with γ_5 matrices in $d \neq 4$ dimensions. *FormTracer* achieves its performance by using FORM as a powerful backend in combination with an advanced decomposition algorithm in Mathematica. Furthermore, a simple but effective way to single out a special time-like direction for finite temperature and density applications in Euclidean field theory is provided. Although developed with specific applications in non-perturbative functional methods in mind, its flexible notation and usability facilitate the use in new and existing general purpose programs, in particular in perturbation theory.

Acknowledgement

This work was done within the fQCD collaboration for which we particularly thank Jan M. Pawłowski. Furthermore, we are grateful to Andreas Rodigast and Jos Vermaseren for many valuable FORM tips and explanations as well as to Vladyslav Shtabovenko for constructive comments especially with respect to γ_5 matrices in general dimensions. We acknowledge discussions with Nicolai Christiansen, Tobias Denz, Aaron Held, Jan M. Pawłowski, Manuel Reichert, and Nicolas Wink.

This work is supported by the grant ERC-AdG-290623, FWF through Erwin-Schrödinger-Stipendium No. J3507-N27, the BMBF grant 05P12VHCTG, the Studienstiftung des deutschen Volkes, the DFG through grant STR 1462/1-1, and in part by the Office of Nuclear Physics in the US Department of Energy's Office of Science under Contract No. DE-AC02-05CH11231.

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