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Code Optimization in FORM

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Abstract

We describe the implementation of output code optimization in the open source computer algebra system FORM. This implementation is based on recently discovered techniques of Monte Carlo tree search to find efficient multivariate Horner schemes, in combination with other optimization algorithms, such as common subexpression elimination. For systems for which no specific knowledge is provided it performs significantly better than other methods we could compare with. Because the method has a number of free parameters, we also show some methods by which to tune them to different types of problems.

1 Introduction

One of the uses of computer algebra is to prepare potentially large formulas for frequent numerical evaluation. This is particularly the case in particle physics. The most widespread way to compute reactions in particle physics is by means of perturbative field theory. Even at the one loop level (usually the second term in the perturbative expansion) one may encouter large numbers of Feynman diagrams, each resulting in a lengthy formula[1]. Such calculations are undertaken to compare theories with experimental results. Hence such formulas have to be integrated over the region of sensitivity of the detectors that measure these reactions. This region is called the experimental acceptance and the only technique that is available to integrate over it is Monte Carlo integration. One may have to evaluate the formulas millions of times to obtain accurate results. Hence it is important to have a representation of the formulas that is as short as possible, even if this involves a non-negligible cost during the computer algebra phase of the calculation.

Optimizing the output of the formulas can be done in two different ways. The first is *domain specific*. This means that specific knowledge about the behavior of the formulas is provided to make the formulas shorter. An example is an equation in two variables x and y, but it is known that $x + y$ and $x - y$ are more natural variables and make the formulas shorter. For the second way either there is no domain specific knowledge, or it is too much work to obtain it. In that case the formula has to be treated by generic means. It should be clear that usually the best results are obtained when domain specific knowledge is applied first, followed by a generic method to clean up what is left.

In computer algebra the challenge is to make a system for the optimization of the output of expressions in the absence of domain specific knowledge. In addition this system should work reasonably fast, which we interpret as subquadratic in the length of the input expression. In the recent past several methods have been published in which two of the authors reported on new techniques to improve upon existing methods [2, 3, 4]. It turns out that an optimization method based on Monte Carlo tree search [5, 6], a recent search method from artificial intelligence and game theory, performs best on the benchmarks that were tested. This method has caused much excitement in the field of game theory, because it has improved the strength of Go playing computer programs from advanced beginner to medium level players, and on small (9x9) boards they have reached top level strength. Application of this technique to the field of formula simplification has led to sufficiently positive results that we have decided to implement it in the computer algebra language FORM [7] in such a way that all its users can benefit from it.

Since this is such a new field, we do not yet have extensive experience with applications and how different types of formulas need different values for the controlling parameters. Hence we have made an implementation in which the user has access to these parameters and can tune them to whole categories of formulas. This means that at the moment we have a number of default settings which may be changed by the user. In later versions we may try to have the program tune these parameters for individual formulas automatically.

The outline of the paper is as follows. In section 2 we explain the algorithms that are used for the simplification. The syntax of the FORM implementation is explained in section 3 including all parameters that can be set. In section 4 we discuss a number of examples.

[1] In special cases other techniques can be used that lead to surprisingly simple formulas [1], but in general these are not applicable.

Section 5 is dedicated to studying the effects of some parameters and the determination of good settings for a number of formulas. We finish with remarks about potential future development. All programs that we use can be obtained from the FORM website at ref.[8].

2 Code optimization algorithms

2.1 Horner's method

For optimizing polynomials in a single variable, the textbook algorithm called *Horner's method* gives an efficient form for evaluating it [9]. It can be written as follows:

$$a(x) = \sum_{i=0}^{n} a_i x^i = a_0 + x(a_1 + x(a_2 + x(\ldots + x \cdot a_n))). \tag{1}$$

If the polynomial is of degree n and dense, this form takes n multiplications and n additions to calculate its value.

It is possible to generalize Horner's method for multivariate polynomials, but this generalization is not unique. First, one of the variables in the polynomial is selected and Eq. (1) is applied, thereby treating the other variables as constants. Next, a different variable is chosen and Horner's rule is applied again on the parts not containing the first variable. This method is repeated until all variables have been selected. As an example, we consider the polynomial $a(x, y, z) = y - 3x + 5xz + 2x^2yz - 3x^2y^2z + 5x^2y^2z^2$ and chose the variable x first, then y and finally z. This results in the following representation:

$$a(x, y, z) = y + x(-3 + 5z + x(y(2z + y(z(-3 + 5z))))). \tag{2}$$

This representation takes 8 multiplications and 5 additions to evaluate, while the original form takes 18 multiplications and 5 additions. This behavior is generic: Horner's method reduces the number of multiplications and leaves the number of additions constant.

For the multivariate Horner method it is important in which order the variables are processed. Different orders may lead to huge differences in the number of operations used to evaluate a polynomial [2]. Classically, simple greedy algorithms like sorting the variables by number of occurrences are used to determine the order [10]. Recently, two of the authors of this paper describedan algorithm based on Monte Carlo tree search to determine more efficient orders [4].

2.1.1 Occurrence order

In the *occurrence order* all variables are ordered with respect to their number of occurrences in the polynomial. The variable that appears most often is the first variable in the order [10]. At every step in the multivariate Horner's method this results in the largest decrease in the number of operations, because it is the most-occurring variable that is factored out of the polynomial. This greedy approach usually gives good results.

Another simple order is the *reverse occurrence order*. As the name suggests, this order contains the variables sorted with respect to the number of occurrences, but with the least-occurring variable first. This method usually results in Horner schemes that use more operations than the normal occurrence order to evaluate the polynomial. However, since the

most-occurring variables are now within the innermost parentheses, more common subexpressions appear, i.e., expressions that appear in multiple places in the polynomial. For the polynomial of Eq. (2) one such common subexpression is $-3 + 5z$.

These common subexpressions can be detected by a method called common subexpression elimination (CSE), see section 2.2, and be calculated beforehand. This algorithm of applying a reverse occurrence order Horner scheme followed by CSE may outperform the analogous algorithm with the normal occurrence order, if lots of common subexpressions exist. The difference in performance between these two algorithms depends primarily on the structure of the input polynomial.

2.1.2 Monte Carlo tree search

Recently, the authors of this paper proposed a method to find more efficient Horner schemes by using Monte Carlo tree search (MCTS) [4]. The different variable orders are represented by a search tree. The root node indicates that no variables have been selected. This root node has n children where n is the number of variables. Traversing down an edge corresponds to choosing a variable. A node at depth d in the tree represents that choices are made for the first d variables in the order. Such a node has $n - d$ children: one for every variable that has not been selected yet. The MCTS method searches through this tree in an asymmetric way, where most-promising branches are traversed first. Fig. 1 shows an example of the traversed part of the MCTS tree after 1 000 iterations while looking for an efficient Horner scheme for a polynomial in 15 variables.

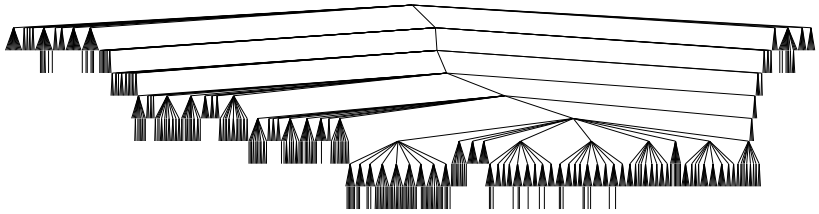

Figure 1: The traversed part of an MCTS tree in the search for a good Horner scheme.

The essence of the MCTS method is the assumption that good solutions are clustered in branches of the search tree. This means that if a reasonable solution is found in one of the branches, there is a good chance that there are more good (and possibly better) solutions in the same branch. Hence, in the case that a reasonable solution is found it may pay to search its neighborhood for better solutions. This is called exploitation. At the same time one should try the untried branches to see whether they have particularly good or bad solutions, because the branches tried so far may not have the best solutions. This process is called exploration. A good MCTS program divides its time between exploiting previously found favorable branches and exploring branches about which little is known.

To determine where to look in the search tree for better solutions several criteria exist. The most-used selection formula is the UCT (upper confidence level for trees) criterion [5],

$$UCT_i = \langle x_i \rangle + 2C_p \sqrt{\frac{2 \log n}{n_i}}, \tag{3}$$

and the child with the highest UCT value is selected. Here $\langle x_i \rangle$ is the average score of child i over the previous traversals, n_i is the number of times child i has been visited before, and n is the number of times the node itself has been visited. C_p is a problem-dependent constant that should be determined empirically.

If one enters a node that has never been visited before, the remaining decisions are all random. This means that one can come to a solution very fast after which one can evaluate the quality of this solution. In the game of Go, for example, this idea of selecting random moves until the game is over and the outcome can the determined might seem like complete madness at first. On the other hand: if there is a good move, one expects that the average score in the branch with this move will be higher than in the other branches and it pays to look a bit better in this branch. Of course there is the risk that a branch with a very good move is missed because an earlier random continuation was particularly bad. Hence one should never exclude branches completely and this is the role of the second term in Eq. (3); eventually the branch will be selected again.

A complete description of MCTS in general and its applications can be found in Ref. [11], while a more detailed description of MCTS for Horner schemes including pseudocode is in Ref. [4].

As mentioned above, for MCTS to work we need clustering of good and bad solutions. Hence the selection of the tree structure is dominantly important. In the case of Horner schemes the choice of whether the outermost variable or the innermost is selected first can make all the difference, in the same way as using occurrence order or reverse occurrence order does. We found that this choice depends on the formula to be optimized. A clear example of this is given in section 5.

2.2 Common subexpression elimination

Large expressions may contain many common subexpressions, in other words, subexpressions that appear in the equation multiple times. A small example of this is the subexpression $-3 + 5z$ in Eq. (2). These can be replaced by a temporary variable to reduce the number of operations, as the following code shows:

$$\begin{aligned} Z_1 &= -3 + 5z \\ a &= y + x(Z_1 + x(y(2z + y(zZ_1)))). \end{aligned} \tag{4}$$

This code uses only 7 multiplications and 4 additions, while the original expression after applying Horner's method uses 8 multiplications and 5 additions.

Common subexpressions can be detected and eliminated by the method of *common subexpression elimination* (CSE) in time linear in the size of the input expression [12]. First, the expression is represented as a binary tree with the operators as inner nodes and the variables and numbers as leaves. The two children of an operator denote its left and right operand. The left panel of Fig. 2 shows an example of a binary expression tree for the polynomial $w^2y + w^2z + wx + wy + wz$.

This expression tree is traversed and each subtree is assigned a number starting with the leaves. Equal subtrees are assigned equal numbers, since these represent common subexpressions. An associative array (e.g., a hash table or balanced binary tree) [13] is used to map subexpressions (i.e., a number, a variable or an operator combined with the identifiers of its two operands) to the identifiers. When moving up in the tree, this map facilitates checking

fast whether a subtree is encountered before or should be assigned a new identifier. The right panel of Fig. 2 shows the labeling of the subtrees after CSE.

This CSE method works particularly well in combination with Horner's method if the variables that appear often in common subexpressions are chosen as innermost variables in the Horner order. In this way, many common subexpressions appear and the cost of evaluation is greatly reduced.

However, this method can also miss many common subexpressions. We consider again the polynomial $w^2y + w^2z + wx + wy + wz$, which can be represented as a binary expression tree in multiple ways of which two of them are shown in Fig. 3. When using CSE, the common subexpression $y + z$ is missed in the right representation, but is detected in the left one. Unfortunately, it seems impossible to detect such structures in time linear in the size of the input expression.

2.3 Greedy optimizations

CSE is not able to detect all forms of common subexpressions as is illustrated by Fig. 3. Therefore another method is needed to detect them and reduce the evaluation cost even further. To do so, equal operators are merged first. Two nodes in the expression tree are merged if they contain equal operators and they are each other's parent and child. The new node has as children all children of merged nodes. Note that the expression tree is not a binary tree anymore after operators are merged. This merging process is shown in Fig. 4.

After merging equal operators the evaluation code is generated. The lines of this code are called *intermediate expressions*. We demand that these intermediate expressions contain only operators of one single type, i.e., either additions or multiplications. Producing code of this form has already been suggested in Ref. [14] for applying Breuer's growth algorithm. The resulting code for the merged tree of Fig. 4 is the left hand side of Eq. (5).

$$\begin{array}{ll} Z_1 = w^2 & Z_1 = w^2 \\ Z_2 = y + z & Z_2 = y + z \\ Z_3 = Z_1 * Z_2 & Z_3 = Z_1 * Z_2 \\ Z_4 = x + y + z \quad \longrightarrow & Z_4 = x + Z_2 \\ Z_5 = w * Z_4 & Z_5 = w * Z_4 \\ a = Z_3 + Z_5 & a = Z_3 + Z_5 \end{array} \tag{5}$$

After writing the code in this way, every expression is scanned through and the number of occurrences of certain small subexpressions is counted. The subexpressions counted are of

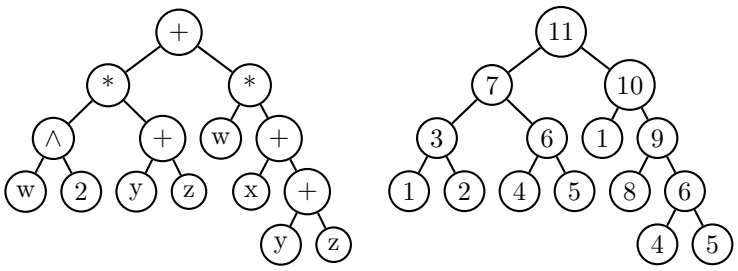

Figure 2: A binary expression tree for the polynomial $w^2y + w^2z + wx + wy + wz$ and the labeling of the nodes after CSE.

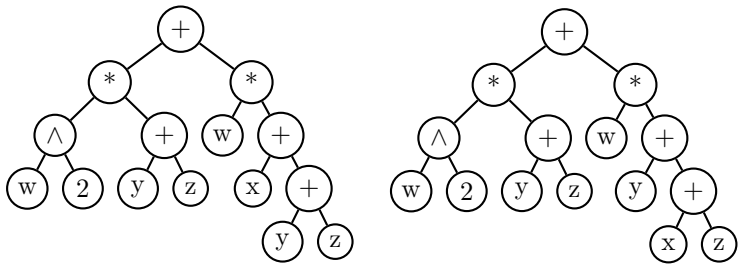

Figure 3: Two different binary expression trees for representing the polynomial $w^2y + w^2z + wx + wy + wz$. Only in the left one, CSE detects the common subexpression $y + z$.

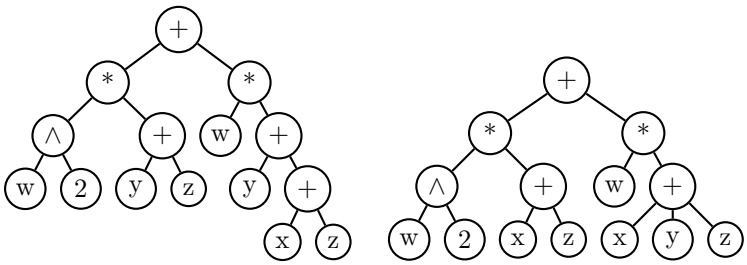

Figure 4: An expression tree of $w^2y + w^2z + wx + wy + wz$ before (left) and after (right) merging operators.

the form

$$x^n, \quad x \cdot y, \quad c \cdot x, \quad x + c, \quad x + y \quad \text{or} \quad x - y. \tag{6}$$

In these small subexpressions x and y are either variables of the polynomial (w, x, y, z in Eq. (5)) or intermediate variables (Z_i in Eq. (5)), and c is a coefficient. For each intermediate expression we loop over all pairs of terms and count the corresponding subexpressions. This takes time proportional to the sum of the squares of the lengths of the intermediate expressions, and is therefore much slower than CSE.

Next, the subexpressions that occur multiple times are determined, because replacing them by new intermediate expressions reduces the total number of operations of the evaluation code. A fraction of these optimizations, that give the largest decrease in evaluation cost, is performed and subsequently a new list of optimizations is generated. This process is repeated until no more optimizations are found.

This algorithm is different from Breuer's growth algorithm [14, 15], where a larger subexpression that generates a bigger decrease in cost is determined. Finding that subexpression is computationally harder than counting our small subexpressions, and this has to be calculated repeatly. We believe the two methods are more or less equivalent though, since the larger substitution may be viewed as a chain of small ones, but have no proof of this.

2.4 Partial factorization

The algorithm of greedy optimizations is good for detecting a lot of common subexpressions. It does not find optimizations of the following form though:

$$\begin{array}{l} Z_1 = x*y*z \\ Z_2 = x*z^2 \\ a = 2*x+y+Z_1+Z_2 \end{array} \quad \longrightarrow \quad \begin{array}{l} Z_1 = y*z \\ Z_2 = z^2 \\ Z_3 = 2+Z_1+Z_2 \\ Z_4 = x*Z_3 \\ a = y+Z_4 \end{array} \tag{7}$$

Here, the variable x is factored out of a number of terms, thereby reducing the number of operations. These kind of optimizations are done by the *partial factorization* method. For each intermediate expression and the intermediate expressions in its operands, the number of occurrences of each variable is counted. If a variable occurs two or more times, the code is optimized analogous to Eq. (7). In our code optimization algorithms, this method of partial factorization is intertwined with the greedy optimizations, so that both methods optimize the evaluation code in turns. This generally gives good resulting code.

This partial factorization method has some similarities with the hypergraph method that performs syntactic factorizations [3]. In this method a polynomial a is factorized as $a = b \cdot c$, such that the number of terms in a is the product of the numbers of terms in b and c. The factors b and c have to be more or less independent for this to happen. In this case the substitution rule of Eq. (7) often finds the corresponding factorization after a few iterations intertwined with the greedy optimizations. This is shown by the sequence underneath.

$$\begin{array}{l} Z_1 = w*y \\ Z_2 = w*z \\ Z_3 = x*y \\ Z_4 = x*z \\ a = Z_1+Z_2+Z_3+Z_4 \end{array} \longrightarrow \begin{array}{l} Z_5 = y+z \\ Z_6 = w*Z_5 \\ Z_7 = y+z \\ Z_8 = x*Z_7 \\ a = Z_6+Z_8 \end{array} \longrightarrow \begin{array}{l} Z_5 = y+z \\ Z_6 = w*Z_5 \\ Z_8 = x*Z_5 \\ a = Z_6+Z_8 \end{array} \longrightarrow \begin{array}{l} Z_5 = y+z \\ Z_9 = w+x \\ a = Z_5*Z_9 \end{array} \tag{8}$$

2.5 Recycling variables

The algorithms to reduce the number of operations (Horner schemes followed by CSE, greedy optimizations and/or partial factorizations) usually result in evaluation code that contains a huge number of intermediate variables, namely one per intermediate expression. Many of them are only used in a small part of the code and can be discarded afterwards. Reusing these variables often greatly reduces the number of temporary variables, which leads to more efficient code and faster compile times when compiling it with traditional compilers.

To generate the final code and recycle the variables, the intermediate expressions are sorted in *depth-first order* [12]. The directed acyclic graph of intermediate expressions is traversed with a depth-first search and an expression is added to the code after all its children are traversed. Next, the life ranges of all expressions are determined by looking at their first and last appearances. Subsequently, new expressions are renumbered to the lowest available number at that stage. This method of renumbering variables is known as *linear scan register allocation* [16] and works much faster for large numbers of variables than the traditional graph coloring algorithms used in many compilers. After appying this final step, the code of Eq. (5)

becomes the following

$$\begin{array}{ll} Z_1 = w^2 & Z_1 = w^2 \\ Z_2 = y + z & Z_2 = y + z \\ Z_3 = Z_1 * Z_2 & Z_1 = Z_1 * Z_2 \\ Z_4 = x + Z_2 \quad \longrightarrow & Z_2 = x + Z_2 \\ Z_5 = w * Z_4 & Z_2 = w * Z_2 \\ a = Z_3 + Z_5 & a = Z_1 + Z_2 \end{array} \tag{9}$$

and only two temporary variables are used to evaluate the polynomial.

3 FORM implementation

3.1 Calling optimization routines

There are several statements that concern the optimization of an expression and its writing. New options of the `Format` statement determine whether optimization is applied and how this is done. Regular output can be printed with the `Print` statement. If the format is set correctly the output is optimized. Such output does not affect the stored version of the expressions that are optimized. It is only the output that takes this representation.

This output, however, is usually not what the user intends. Things are different when the `#optimize` instruction is used. This optimizes a single expression and replaces the original formula by the new one and keeps all temporary statements like the ones in the r.h.s. of Eq. (9) in memory. This can only be done for one expression at a time. As soon as a second expression is optimized the results of the previous optimization are lost and so is the entire previous expression. The reason for this behavior is explained below. The optimized expression and its supportive statements can be written to the standard output or a file with the `#write` instruction. This last method is very powerful and allows the automatic construction of complete programs.

The `#write` instruction has in the format string the new specifier `%O` which writes the intermediate statements that are prepared by the most recent `#optimize` instruction. It uses the current format settings (as for fortran or C) and the current settings for the extra symbols. Additionally, when for instance `%5O` is specified, all lines in the output will have 5 spaces at the start of the line. The format specifier `%E` can write the optimized expression.

To declare the array for the temporary variables, the user can access the maximum and minimum range of the array used in the optimized code by the preprocessor variables `optimmaxvar_` and `optimminvar_`, respectively.

Finally, there is a `#clearoptimize` instruction that clears the optimization buffer and removes the optimized expression.

If an expression contains brackets, the outsides of the brackets are not treated in the optimizations. This can be used to create simultaneous optimizations as in the second example in the next section.

3.2 Interaction with extra symbols

Some operations in FORM have been implemented only for multivariate polynomial expressions and the same may hold for some procedures that have been constructed by users. To facilitate this FORM version 4.0 has been equipped with the statement `ToPolynomial` that replaces all objects (like functions or dotproducts) by system defined symbols, called extra

symbols. It is also possible to undo this substitution at a later stage with the `FromPolynomial` statement. The `ExtraSymbol` statement controls the output representation of the extra symbols in the case they have to be printed.

The implementation of code optimization needs the notion of systems defined intermediate variables. We define these temporary variables as extra symbols in addition to the ones that may exist already.

The definitions of the extra symbols that are introduced by the `ToPolynomial` statement are unique as in

```
Z1_ = g(x)
Z2_ = g(y)
Z3_ = f(x)
```

and hence we can store them in rather simple and semi permanent buffers.

The intermediate variables introduced during optimization can be reused as we explained before and hence the definitions of the corresponding extra symbols are not unique as in

```
Z1_=x + y;
Z2_=y*Z1_;
Z1_=Z1_ + z;
Z1_=z*Z1_;
Z3_=x^2;
Z1_=Z1_ + Z3_ + Z2_;
F=2*Z1_;
```

where the definitions of `Z1_` and `Z2_` are overwritten (in the case of `Z1_` even more than once). This, in combination with the potential number of generated statements is the reason that this category of extra symbols is stored in a different, more temporary way. We allocate a special buffer for them and because of its potential size, we do not want to allocate more than a single buffer. If there would be more than a single one, there would be additional complications concerning the numbering of the variables in the different buffers: are they independent, causing several instances of `Z1_`, or should they be numbered consecutively? We have opted for a single buffer, but with a mechanism for optimization of more than one object at the same time.

3.3 Optimization options of the Format statement

The `Format` statement has a number of options to control the code optimization. The easiest to use are the following:

O0 Switches off all optimizations and prints the output the normal FORM way. This is the default.

O1 Activates the lowest level of optimization. It is very fast, i.e., linear in the size of the expression, and gives reasonably efficient code.

O2 Activates the medium level of optimization. This is slower than the previous setting, but usually gives better results.

O3 Activates the highest level of optimization. It can be rather slow, but usually gives even better results.

These levels of optimization refer to some default settings of all controlling parameters. These default values are in Tab. 1. It is also possible to set each parameter individually to fine-tune the optimization process. The parameters that can be set are divided in several categories. First, it is possible to set which Horner schemes are tried:

Horner=(Occurrence | MCTS) Determines whether a (possibly reverse) occurrence order Horner scheme is used or whether MCTS is employed to find Horner schemes.

HornerDirection=(Forward | Backward | ForwardOrBackward | ForwardAndBackward) For the occurrence order, forward selects the normal one and backward selects the reverse one. ForwardOrBackward and ForwardAndBackward try both. For MCTS, forward starts selecting the first variables in the Horner scheme and backward starts with the last ones. ForwardOrBackward tries both of these schemes. ForwardAndBackward fill the order from both sides simultaneously, resulting in more options, but also a much larger search tree.

In the case of MCTS there are various parameters that can control the search process:

MCTSConstant=<*value*> This is the constant C_p in Eq. (3).

MCTSNumExpand=<*value*> The number of times the tree is traversed and hence the number of times that a Horner scheme is constructed.

MCTSNumKeep=<*value*> The number of best solutions that will be remembered.

MCTSNumRepeat=<*value*> As we will see in the section 5 sometimes it is more advantageous to run a new tree search several times, each with a smaller number of expansions. This parameter tells how many times we will run with a new tree. The total number of tree traversals is the product of MCTSNumRepeat and MCTSNumExpand.

MCTSTimeLimit=<*value*> The maximum time in seconds that is used when searching through the tree.

The Horner methods generate a number of Horner schemes: one or two in the case of occurrence order schemes, depending of the direction parameter, and a number equal to MCTSNumKeep in the case of MCTS. Next, for each stored Horner scheme other optimizations are performed as determined by the following parameter:

Method=(None | CSE | Greedy | CSEGreedy) Determines what method is used for optimizing the generated Horner schemes. CSE performs common subexpression elimination (see section 2.2) and Greedy performs greedy optimizations (see section 2.3). CSEGreedy performs CSE followed by greedy optimizations; usually this is somewhat faster than just greedy optimizations, but it gives slightly worse results. The option None does nothing after applying the Horner scheme and is only useful for debugging purposes.

When the method of greedy optimizations is used, repeatedly all optimizations are determined and a few of them are performed. The following parameters are used to tune the greedy method:

GreedyMaxPerc The percentage of the possible optimizations that is performed.

GreedyMinNum The minimum number of possible optimizations that is performed.

GreedyTimeLimit The maximum time in seconds that is spent in the process of greedy optimization.

Experimentation shows that the influence of the first two parameters is not very big. They might however be useful when the greedy method is expanded with the recognition of more complicated substructures.

Additionally, there are two more general settings:

Stats=(On | Off) This parameter determines whether statistics of the optimization are shown.

TimeLimit=<*value*> This set both the MCTSTimeLimit and the GreedyTimeLimit to half of the given value.

Finally there are a few options that can help very much with debugging:

DebugFlag=(On | Off) In the case that the value is On, the list of temporary variables is printed in reverse order with the the string "id " in front. This makes them into a set of FORM substitutions that undo the optimizations. One can use this for instance to make sure that the optimized code is identical to the original.

PrintScheme=(On | Off) This option (when On) will print the Horner scheme. That is the order in which the variables were taken outside parentheses.

Scheme=(list of symbols) The list should be enclosed by parentheses and the symbols should be separated by either blanks or comma's. This option will fix the Horner scheme to be used.

All options should be specified in a single format statement and be separated either by commas or blank spaces. When `Format Optimize` is used, first the default settings are taken and then the options that are specified overwrite them. It is allowed to have the O1, O2, O3 optimization specifications followed by options. In that case the program first sets the values of those specifications and then modifies according to what it encounters in the rest of the statement.

4 Examples

4.1 Optimizing a single expression

The first example shows a rather simple use.

	O1	O2	O3 (default)
Horner	occurrence	occurrence	MCTS
HornerDirection	OR	OR	OR
MCTSConstant	—	—	1.0
MCTSNumExpand	—	—	1000
MCTSNumKeep	—	—	10
MCTSNumRepeat	—	—	1
MCTSTimeLimit	—	—	0
Method	cse	greedy	greedy
GreedyMinNum	—	10	10
GreedyMaxPerc	—	5	5
GreedyTimeLimit	—	0	0
Stats	off	off	off
TimeLimit	0	0	0

Table 1: Values for the various parameters in the predefined optimization levels. OR stands for ForwardOrBackward.

```
    Symbols x,y,z;
    Off Statistics;
    Local F = 6*y*z^2+3*y^3-3*x*z^2+6*x*y*z-3*x^2*z+6*x^2*y;
    Format O1,stats=on;
    Print;
    .end
      Z1_=y*z;
      Z2_= - z + 2*y;
      Z2_=x*Z2_;
      Z3_=z^2;
      Z1_=Z2_ - Z3_ + 2*Z1_;
      Z1_=x*Z1_;
      Z2_=y^2;
      Z2_=2*Z3_ + Z2_;
      Z2_=y*Z2_;
      Z1_=Z2_ + Z1_;
      F=3*Z1_;
*** STATS: original  1P 16M 5A : 23
*** STATS: optimized 0P 10M 5A : 15
```

The statistics show that we started with 23 operations (one power which counted double because it was a third power, 16 multiplications and 5 additions) and that we are left with 15 operations. Note that squares are counted like a single multiplication. If we run this program with the option O2 we obtain

```
      Z1_=z^2;
      Z2_=2*y;
      Z3_=z*Z2_;
      Z2_= - z + Z2_;
      Z2_=x*Z2_;
```

```
      Z2_=Z2_ - Z1_ + Z3_;
      Z2_=x*Z2_;
      Z3_=y^2;
      Z1_=2*Z1_ + Z3_;
      Z1_=y*Z1_;
      Z1_=Z1_ + Z2_;
      F=3*Z1_;
*** STATS: original  1P 16M 5A : 23
*** STATS: optimized 0P 9M 5A : 14
```

and with O3 we have

```
      Z1_=x + z;
      Z2_=2*y;
      Z3_=Z2_ - x;
      Z1_=z*Z3_*Z1_;
      Z3_=y^3;
      Z2_=x^2*Z2_;
      Z1_=Z1_ + Z3_ + Z2_;
      F=3*Z1_;
*** STATS: original  1P 16M 5A : 23
*** STATS: optimized 1P 6M 4A : 12
```

It is possible to obtain an even better decomposition, but this requires simplifications of the type $x^2 + xz + z^2 \to (x + z)^2 - xz$ which is not within the scope of the simplifications we apply. Similarly $x^2+2xz+z^2$ will not be seen as a square. Such simplifications require entirely different algorithms which should be executed before the FORM algorithms are applied.

4.2 Simultaneous optimization

Imagine we have to compute two objects F and G. If we can compute the common subexpressions of both only once we may save much. To do this we put the two expressions into a single expression H in such a way that we can separate them again by bracketting in the extra variable u. If the expression is bracketted in terms of u at the moment of optimization FORM will know that it is not allowed to combine terms like `u*a+u^2*a` into `(u+u^2)*a`. The output expression in H still contains the variable u and when we bracket again in u, we can recover the individual expressions, but now in their optimized version.

```
Symbols x,y,z,u;
ExtraSymbols,array,tmp;
Off Statistics;
Local F = (x+y+z)^2;
Local G = (x+2*y+z)^2;
.sort
Format O3;
Local H=u*F+u^2*G;
B u;
.sort
#optimize H
```

```
    B u;
    .sort
    Local F1 = H[u];
    Local G1 = H[u^2];
    .sort
    #write <> "%5O"

     tmp(1)=z + 2*x;
     tmp(1)=tmp(1)*z;
     tmp(2)=x^2;
     tmp(1)=tmp(1) + tmp(2);
     tmp(2)=z + x;
     tmp(3)=2*tmp(2) + y;
     tmp(3)=y*tmp(3);
     tmp(3)=tmp(3) + tmp(1);
     tmp(2)=y + tmp(2);
     tmp(2)=y*tmp(2);
     tmp(1)=4*tmp(2) + tmp(1);

    #write <> "\n     F=%e     G=%e",F1,G1

     F=tmp(3);
     G=tmp(1);

    .end
```

The same program, but now without writing the output and showing statistics, also for the optimization of the individual expressions, shows the gain by doing the optimization simultaneously.

```
    Symbols x,y,z,u;
    ExtraSymbols,array,tmp;
    Off Statistics;
    *Format nospaces;
    Local F = (x+y+z)^2;
    Local G = (x+2*y+z)^2;
    .sort
    Local H=u*F+u^2*G;
    B u;
    *Print;
    .sort
    Format O3,stats=on;
    #optimize H
*** STATS: original  0P 19M 10A : 29
*** STATS: optimized 0P 7M 7A : 14
    .sort
    #optimize F
*** STATS: original  0P 9M 5A : 14
```

```
*** STATS: optimized 0P 5M 5A : 10
    #optimize G
*** STATS: original  0P 10M 5A : 15
*** STATS: optimized 0P 5M 5A : 10
    .end
```

The counting of the number of operations in the original version of H takes into account that the brackets fulfil a special role here.

Of course, by using factorization one can write the above expressions shorter than this, but that is not the point here. In general we do not apply factorization because that succeeds only in very rare cases and it can be very slow on large expressions. Potential factorization is considered 'domain specific' and falls under the responsibility of the user.

4.3 Optimizing resultants

The third example is bigger. It comes from ref. [3]. We compute the resultant of two polynomials $A = \sum_{i=0}^{m} a_i x^i$ and $B = \sum_{i=0}^{n} b_i x^i$. This is a $(m+n) \times (m+n)$ determinant and gives a polynomial in $m+n+2$ variables. The program is rather short and can go to rather large values of m and n. The complete program can be picked up from the FORM website (see ref [8]). Here we show the final part of the program in which F is a stored expression containing the 7×5 resultant:

```
Format O1,stats=on;
L F1 = F;
.sort
#message CPU time till now: 'time_' sec.
#optimize F1
.store
Format O2,stats=on;
L F2 = F;
.sort
#message CPU time till now: 'time_' sec.
#optimize F2
.store
Format O3,stats=on,mctsconstant=0.1;
L F3 = F;
.sort
#message CPU time till now: 'time_' sec.
#optimize F3
.store
#message CPU time till now: 'time_' sec.
.end
```

and the output is

```
~~~CPU time till now: 0.34 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 41P 11745M 8359A : 20210
~~~CPU time till now: 0.75 sec.
```

```
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 42P 8873M 7417A : 16398
~~~CPU time till now: 6.12 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 25P 5551M 5561A : 11171
~~~CPU time till now: 189.73 sec.
  189.73 sec out of 189.79 sec
```

The times are on an Opteron 2.6 GHz processor. The first time is the time needed to obtain the 12×12 determinant. The times are cumulative. It is possible to obtain even better values at the cost of more CPU time. It is also possible to run the program with TFORM or PARFORM to get the benefit of parallelization. For the O1 and O2 optimizations this gives a modest improvement in the time, because it runs the scheme twice: once with the Horner scheme in forward mode and once in backward mode (as in the forwardorbackward setting). These can be executed in parallel. The Monte Carlo approach of the O3 level is very suitable for parallelization. This is illustrated by the following TFORM run with 4 workers:

```
~~~CPU time till now: 0.86 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 41P 11745M 8359A : 20210
~~~CPU time till now: 1.47 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 42P 8873M 7417A : 16398
~~~CPU time till now: 7.17 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 25P 5306M 5364A : 10730
~~~CPU time till now: 220.27 sec.
  0.37 sec + 220.00 sec: 220.38 sec out of 58.81 sec
```

The times printed during the running are the times of the master processor and hence rather meaningless. But the final time involves all workers and the 58.81 sec is the real time that passed. The difference between the total CPU time of the sequential run (189.79 sec) and the run with 4 workers (220.38 sec) is partially due to overhead and partially to bus-congestion. Yet it is clear that we gain more than a factor 3. The different number of operations in the O3 optimization is due to the Monte Carlo nature and the fact that each worker has its own initialization of the random number generator. In general such multicore runs are not deterministic anyway, because the order in which objects are processed is not fixed. For regular algebra this is only noticed in the intermediate statistics of a module (not in the answer of course), but here it becomes a real effect.

A good demonstration of the statistical nature is when we run the same program on 24 workers:

```
~~~CPU time till now: 1.07 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 41P 11745M 8359A : 20210
~~~CPU time till now: 1.65 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 42P 8873M 7417A : 16398
```

```
~~~CPU time till now: 7.39 sec.
*** STATS: original  12044P 106580M 11379A : 142711
*** STATS: optimized 23P 6331M 6003A : 12388
~~~CPU time till now: 376.19 sec.
  0.32 sec + 376.25 sec: 376.58 sec out of 23.07 sec
```

Suddenly the final answer has 12388 operations. We also see that the total CPU time has increased enormously. As far as we can tell this is bus-congestion. It also shows that running with very many workers does not always give correspondingly better execution times.

4.4 Physics examples

For the purpose of 'realistic' testing we have taken three formulas that were generated by the GRACE [17, 18] system which generates matrix elements for the product of one loop graphs and tree graphs. Each formula represents a diagram and the whole is written in terms of Feynman parameters. The coefficient of each combination of Feynman parameters is to be evaluated numerically and put in an array. A separate routine will then compute the corresponding integrals and multiply them by these coefficients. This means that the best procedure is to optimize these coefficients simultaneously.

The first formula comes from the reaction $e^+e^- \to e^+e^-\gamma$ and concerns a loop diagram with a 5-point function. In total there are 5717 terms, containing a total of 15 different symbols, which includes the 4 Feynman parameters. We call this formula HEP(σ). A straightforward evaluation takes 47424 mathematical operations. For this example we do not do a simultaneous optimization. We just do a global optimization, including the Feynman parameters, just to see how this type of formulas can be improved. It made it also easier to create an output for quick testing with compilers.

The other two formulas are called F_{13} and F_{24} and come from the reaction $e^+e^- \to \mu^+\mu^- u\overline{u}$ and are diagrams with a 6-point function. The F_{13} formula contains 105114 terms, 5 Feynman parameters and 24 other variables. Its direct evaluation takes 1 068 153 mathematical operations. The F_{24} formula contains 836010 terms, 5 Feynman parameters and 31 other variables. It needs 7 722 027 mathematical operations in its raw version. Both formulas have 56 different combinations of Feynman parameters.

4.5 Comparison with other algorithms

We have compared the current implementation with results from the literature and programs we had access to.

4.6 Compiled results

Because the object of the code optimization is to create numerical programs that will be shorter and faster, we also have a look at what the compiler can make of the code. To do this in a fair way, we must take into account that the pow function in C is rather inefficient. It needs two double arguments and then becomes very slow. Hence we made a function that takes a double and an integer argument, and put it in the same file as the optimized code. This way the compiler can make inline code and optimize better. For the FORM optimized code this makes hardly any difference as there are very few calls to the power function. For the original formula however it makes a difference of more than a factor 10. The results are

	7-4 resultant	7-5 resultant	7-6 resultant	HEP(σ)
Original	29163	142711	587880	47424
FORM O1	4968	20210	71262	6099
FORM O2	3969	16398	55685	4979
FORM O3	3015	11171	36146	3524
Maple	8607	36464	-	17889
Maple tryhard	6451	$\mathcal{O}(27000)$	-	5836
Mathematica	19093	94287	-	38102
HG + cse	4905	19148	65770	-
Haggies(Ref. [19])	7540	29125	-	13214

Table 2: Number of operations after optimization by various programs. The number for the 7-5 resultant with 'Maple tryhard' is taken from ref [3]. For the 7-4 resultant they obtain 6707 operations, which must be due to a different way of counting. The same holds for the 7-6 resultant as ref [3] starts with 601633 operations. The FORM O3 run used $C_p = 0.07$ and 10×400 tree expansions.

in Tab. 3. All times were on a 3.2 GHz Xeon laptop and were obtained by evaluating the function 10^6 times.

	Format O0	Format O1	Format O2	Format O3
gcc -O0	83.543	11.266	10.200	6.757
gcc -O1	14.400	5.278	4.664	3.171
gcc -O2	17.091	5.880	5.266	3.498
gcc -O3	17.119	5.686	5.006	3.302

Table 3: Execution times for the resulting C code of the physics formula HEP(σ) in microsec. The O3 option in FORM used $C_p = 0.8$ and 3000 tree expansions. It produced 3358 terms.

We have also created the outputs in FORTRAN and made a similar table (4).

	Format O0	Format O1	Format O2	Format O3
gfortran -O0	54.687	11.243	10.192	6.796
gfortran -O1	17.320	5.679	4.997	3.341
gfortran -O2	17.382	5.689	5.044	3.318
gfortran -O3	17.336	5.676	5.020	3.318

Table 4: Execution times for the resulting FORTRAN code of the physics formula HEP(σ) in microsec. The formulas were as in Tab. 3.

It is interesting to note that in all cases the O1 option of the (GNU) C compiler gives the fastest code. In the case of the gfortran compiler this effect does not exist.

Of course the optimizer of the compilers is not allowed to use certain optimizations that we can use. A compiler is not allowed to assume that addition is associative in order to not upset programs that have been coded carefully to avoid numerical instabilities or overflow problems.

On the whole there is not much difference between the C and the FORTRAN code, provided we manage to have the (low) powers made inline in the C code. FORTRAN does

this automatically.

Finally we present the corresponding table for the 7-6 resultant. This is a much bigger expression and we include the running times of both FORM and the GNU C compiler. We can

	Format O0	Format O1	Format O2	Format O3
Operations	587880	71262	55685	36146
FORM time	0.12	1.66	65.43	2398
gcc -O0 time	29.02	6.33	5.64	3.36
run	119.66	13.61	12.24	7.52
gcc -O1 time	5098.8	295.96	199.47	92.09
run	26.98	6.88	6.12	3.80
gcc -O2 time	4891.5	247.60	163.79	74.15
run	21.87	7.00	6.22	3.80
gcc -O3 time	4910.4	276.77	179.24	79.11
run	21.89	6.95	6.19	3.84
gcc -O1 time	3018.6	295.96	199.47	80.82
run	24.30	6.88	6.12	3.58
gcc -O2 time	3104.4	247.60	163.79	65.21
run	21.09	7.00	6.22	3.93
gcc -O3 time	3125.4	276.77	179.24	71.02
run	21.02	6.95	6.19	3.93

Table 5: FORM run time, compilation times and the time to evaluate the compiled formula 10^5 times (run). All times are in seconds. The O3 option in FORM used $C_p = 0.07$ and 10×400 tree expansions. The top compilations are with the powers taken as macro's and the last three 'lines' with the powers as inline functions.

see from the table that an optimal sum-time depends on the number of formula evaluations[2]. In all cases however one of the FORM optimizations will give the best result. It should be noted that for this formula the O1 option of the compiler does not always produce the fastest code.

5 Effects of the parameters

5.1 Scatter plots

In this section we will study a few expressions and how the various parameters can influence the results of the optimization process. Because the MCTS process involves random numbers, the final answer is not always the same. We show this by means of scatter plots. In order to create scatter plots we have implemented an extra random number generator. FORM has already the regular function `random_`, but this function generates random integers. For the scatter plots we needed random values for the parameter C_p in Eq. (3). These should be floating point numbers and follow a distribution. Unfortunately, currently FORM does not have floating point numbers and the algebraic expressions do not tolerate them. Hence the only way we can carry floating point numbers around is as strings. This dictates that the

[2]For this article we ignore the fact that the fastest evaluation would be to compute the original 13×13 determinant which, considering the zeroes, would take just a few hundred operations.

preprocessor should handle them for now. Therefore we have created a preprocessor variable `random_` which takes three arguments as in

```
#define R "‘random_(log,0.01,10.0)’"
```

which stores a floating point value in the preprocessor variable R. The generation is with a logarithmic distribution and the number will be between 0.01 and 10.0. Internally it uses of course the same random number generator as the `random_` function. Hence it is affected in the same way by the `#setrandom` instruction.

Currently the `random_` preprocessor variable can generate according to two distributions: logarithmic (log) and linear (lin). There might be more in the future if there is a demand for it. At the moment the only place where they can be used is in the `Format Optimize` statement for the `MCTSConstant` option. People who would like to install their own distributions should look at the function PreRandom in the source file reken.c.

5.2 Effects of MCTSconstant, MCTSnumexpand and hornerdirection

In the first plots we show the result for HEP(σ), which is the same expression as in section 4.4, generated with the GRACE system. We take a random value for the constant C_p and run the optimization for a given number of points. The final number of operations in the output determines the ‘answer’ and it constitues one dot in the scatter plot. The program looks like

```
Symbol amel2 zk xcp3 xcp1 x1 x5 x4 xcp2 x3
            e2e1 e3e2 e3e1 e4e2 e4e1 EFUN;
Off Statistics;
.global
#include- ReadSigma.h
.store
#setrandom 1021
#do i = 1,4000
  #redefine R "‘random_(log,0.01,10.0)’"
  #message mctsconstant = ‘R’
  Format O3,mctsconstant=‘R’,
         hornerdirection=backward,
         method=cse,mctsnumexpand=3000,stats=on;
  L       FF = Sigma;
  .sort
  #Optimize FF
  .store
#enddo
.end
```

The file ReadSigma.h contains the expression and is more than 5000 lines long. Running the program with TFORM can speed it up considerably. Alternatively one could run various instances of the program, each with a different initialization of the random number generator and with a smaller number of iterations in the loop. The output would look like

```
~~~mctsconstant = 1.482771
*** STATS: original  1270P 39168M 5716A : 47424
```

```
*** STATS: optimized 2P 1995M 2123A : 4122
~~~mctsconstant = 0.073660
*** STATS: original  1270P 39168M 5716A : 47424
*** STATS: optimized 2P 1916M 2287A : 4207
~~~mctsconstant = 0.135939
*** STATS: original  1270P 39168M 5716A : 47424
*** STATS: optimized 3P 1893M 2198A : 4097
                    .
                    .
                    .
```

and so on.

Let us first look at what happens when we vary the number of tree expansions. In Fig. 5 we see scatter plots for 4 different values: 300, 1000, 3000 and 10000 expansions.

At the right side (larger values of C_p) of the plots we see a rather diffuse distribution. When C_p is large, exploration is dominant, which means that at each time we try a random (new) branch and knowledge about the quality of previously visited branches is more or less ignored. On the left side there is quite some structure. Here we give a large weight to exploitation: we prefer to go to the previously visited branches with the best results. Branches that previously had a poor result may never be visited again. This means that there is a big chance that we end up in a local minimum. The plots show indeed several of those (the horizontal bands). When there is a decent balance between exploration and exploitation it becomes very likely that the program will find a good minimum. The more points we use the better the chance that we hit a branch that is good enough so that the weight of exploitation will be big enough to have the program return there. Hence we see that for more points the value of C_p can become bigger. We see also that at the right side of the plots using more evaluations gives a better smallest value. This is to be expected on the basis of statistics. In the limit that we ask for more evaluations than there are leafs in the tree we would obtain the best value.

Clearly the optimum is that we tune the value of C_p in such a way that for a minimum number of expansions we are still almost guaranteed to obtain the best result. This depends however very much on the problem. In the case of the formula of Fig. 5 this would be $C_p = 0.7$.

The HEP(σ) formula gives the best results when we use backward as the value for the hornerdirection parameter. This is what we used for Fig. 5. In the case we use forward for this parameter we obtain Fig. 6. Comparing the two figures shows that the first has the better potential to give an optimal result. It reflects the fact that the backward option gives a better yield of common subexpressions. This can depend very much of the problem as we will see.

With the resultants we have the opposite effect as shown in Fig. 7. Here the backward direction is far from ideal and the forward direction works well, provided we go through the tree a sufficient number of times.

The effect of the forward/backward selection shows the importance of selecting the proper tree structure for the problem. The more the good leaves are clustered on few branches, the better the MCTS can work. Because of the big difference between the forward/backward selections the normal reaction is to set the defaults to trying both orderings. In the case of Fig. 8 for the HEP(σ) formula this obtains close to optimal results. Of course a percentage of points will be wasted by using the wrong direction and hence we see the random r.h.s. in the graphs move a little bit to the left. In Fig. 7 this is unfortunately counterproductive. This

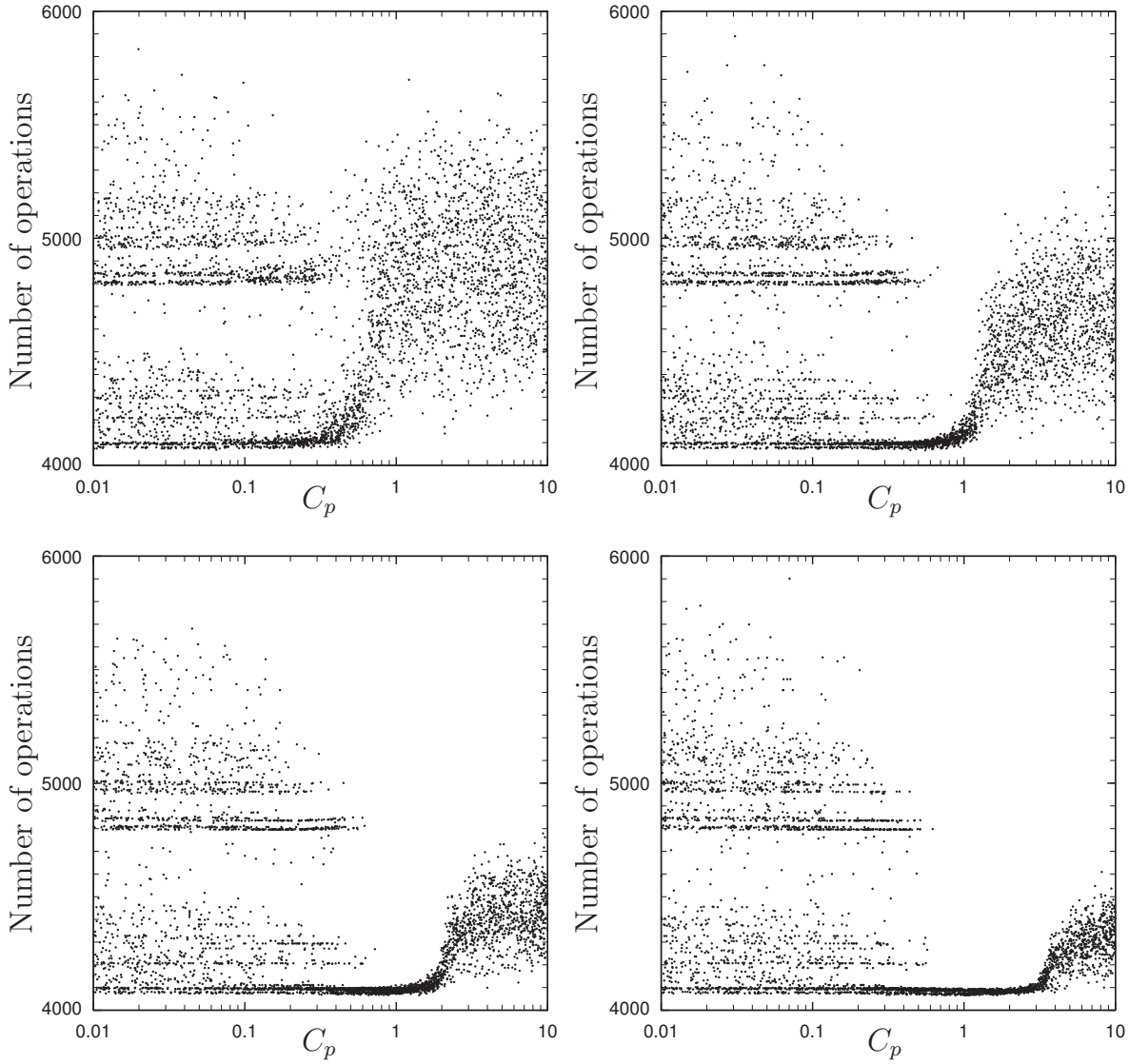

Figure 5: Scatter plots for 300, 1000, 3000, 10000 points per MCTS run. Each plot has 4000 runs. The formula optimized is one obtained from a physics program (HEP(σ)) as explained in the text.

shows that once one knows the best direction for the problem at hand it is better to specify it. This will give a better efficiency. As the plots show a number of runs with a small number of points and relatively few tree expansions should indicate what is the best direction.

5.3 Effect of MCTSnumrepeat

If we take another look at Fig. 5 we notice that in the left sides the distributions are nearly identical, independent of the number of tree expansions. This suggests a new approach: if, instead of 3000 expansions in a single run, we take, say, 3 times 1000 expansions and take the best result of those, the left side of the graphs should become far more favorable. This is illustrated in Fig. 9. We notice a number of things here: when each run has too few points, we

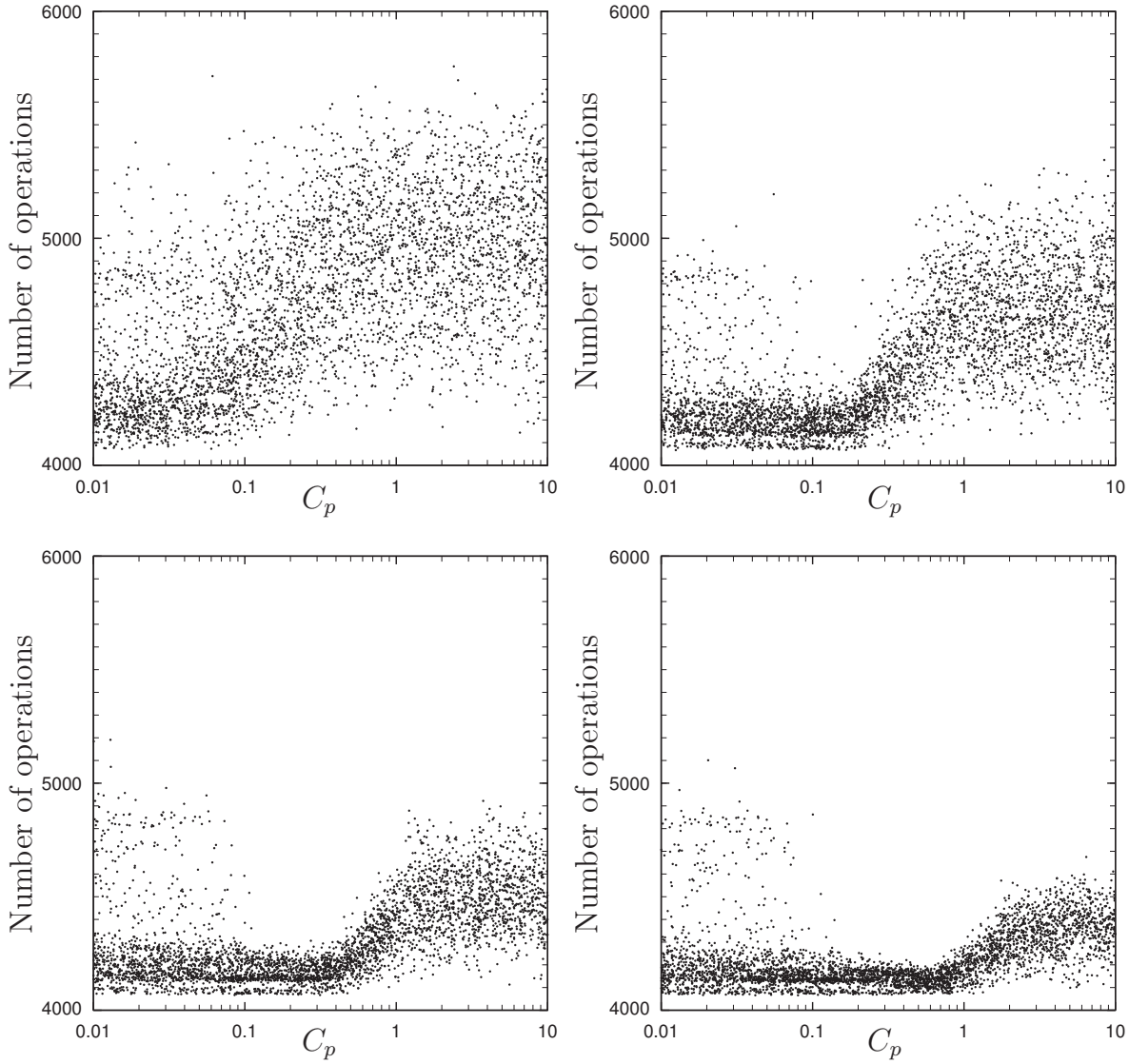

Figure 6: Scatter plots for 300, 1000, 3000, 10000 points per MCTS run. Each plot has 4000 runs. The formula optimized is HEP(σ) as explained in the text. Here we use the value 'forward' for the hornerdirection parameter.

do not find a good local minimum and in the limit of runs of a single point per run the results revert to that of the almost random branches for large values of C_p. The multiple runs make us loose the beautiful minimum near $C_p = 0.7$, because we do not have a correllated search of the tree. If, however,we have no idea what would be a good value for C_p it seems best to select a value that is small and make multiple runs as used here, provided that the number of expansions is big enough for finding a decent local minimum in a branch of the tree. At this point it should be remarked that TFORM and PARFORM will give a result that is statistically a little bit inferior to a run with sequential FORM and the same number of tree expansions. In the case of sequential FORM each tree expansion takes all previous tree expansions into account, while in the cases of TFORM and PARFORM a new tree expansion has no access to

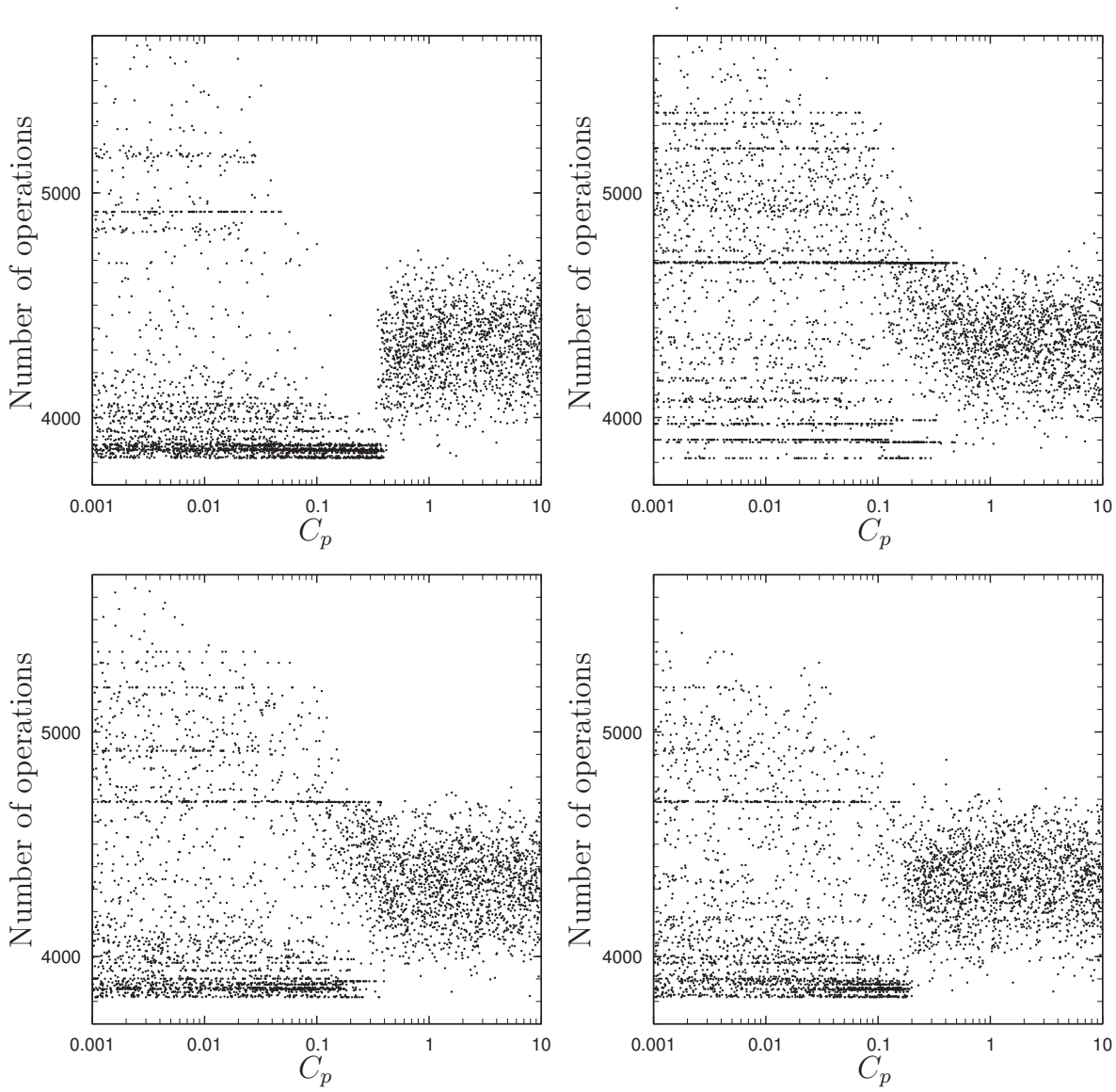

Figure 7: Scatter plots for 5000 points per MCTS run. Each plot has 4000 runs. We optimize the 7-4 resultant as explained in the text. The top left plot is with the forward direction and the top right plot is with the backward direction for the horner scheme. The bottom left plot is for the forwardorbackward direction and the bottom right plot is for the forwardandbackward direction.

the expansions that are still in progress inside other workers. This is particularly relevant when one uses many runs each with a small number of points.

The next question is: "What is a good value for the number of tree expansions per run?" We investigate this in Fig. 10. We select a small value for C_p (0.01) and run for several values of the total number of tree expansions. The calculations in the left graph are for the formula HEP(σ) and in the right graph for the 7-4 resultant. The minima for HEP(σ) coincide more or less around 165 expansions per tree and for the 7-4 resultant around 200 expansions per tree.

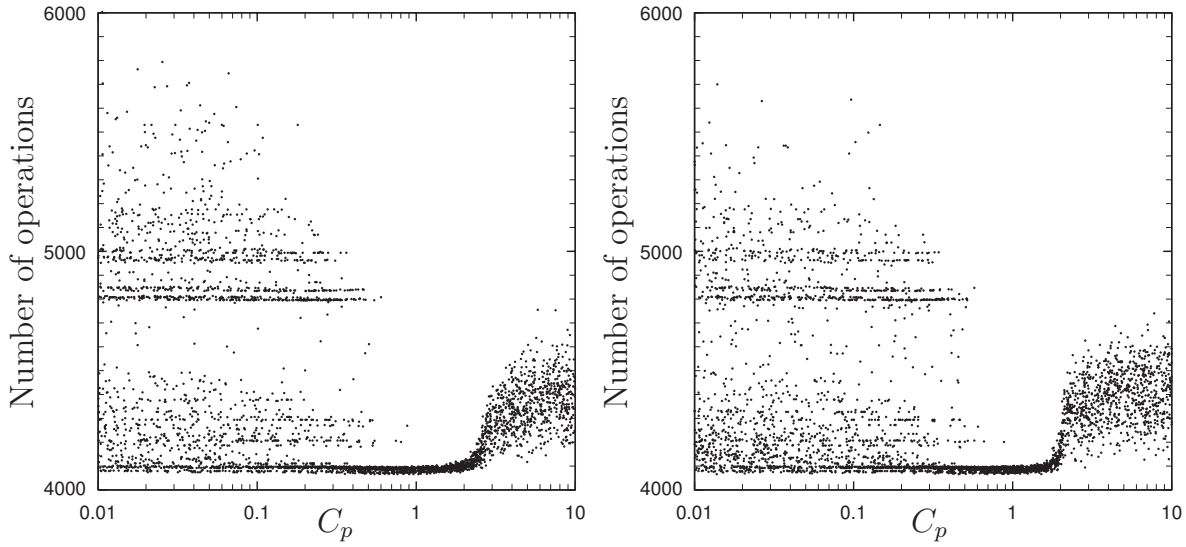

Figure 8: Scatter plots for 5000 points per MCTS run. Each plot has 4000 runs. The formula optimized is HEP(σ) as explained in the text. The left plot is with the backwards direction and the right plot is with the forwardorbackward option (default).

We believe this to be correlated with the square of the number of variables. To saturate the nodes around a single path takes $\frac{1}{2}n(n+1)$ expansions. The remaining expansions are used to search around this path and are apparently enough to find a local minimum. The right top plot of Fig. 9 was selected with 18 trees of 167 expansions per tree with this minimum in mind. For this formula this seems to be the optimum if one does not know about the value $C_p = 0.7$ or if one cannot run with a sufficient number of expansions to make use of its properties.

We have also made a few runs for the 7-5 and 7-6 resultants and find minima around 250 and 300 respectively. This suggests that if the number of variables is in the range of 13 to 15 a good value for the number of expansions is 200-250 and this will then be multiplied by the value of MCTSNumRepeat to obtain a good total number of tree expansions.

Similar studies of other physics formulas with more variables ($\mathcal{O}(30)$) show larger optimal values for the number of expansions per run and less pronounced local minima. Yet also here many smaller runs can give better results than a single big run, provided that the runs have more than a given minimum number of tree expansions.

In the above examples we have intentionally omitted the greedy optimizations because they slow the programs down and do not make qualitative changes in what we wanted to demonstrate. This can be seen in Fig. 11 in which we show typical results with the greedy optimizations included.

The plots show clearly the same behaviour as the plots without the extra greedy optimizations. The formulas are just 15-25% shorter.

6 Further improvements

As we have mentioned before, it may pay to spend some attention to the formulas before sending them to the FORM optimization. One generic improvement one may think about is

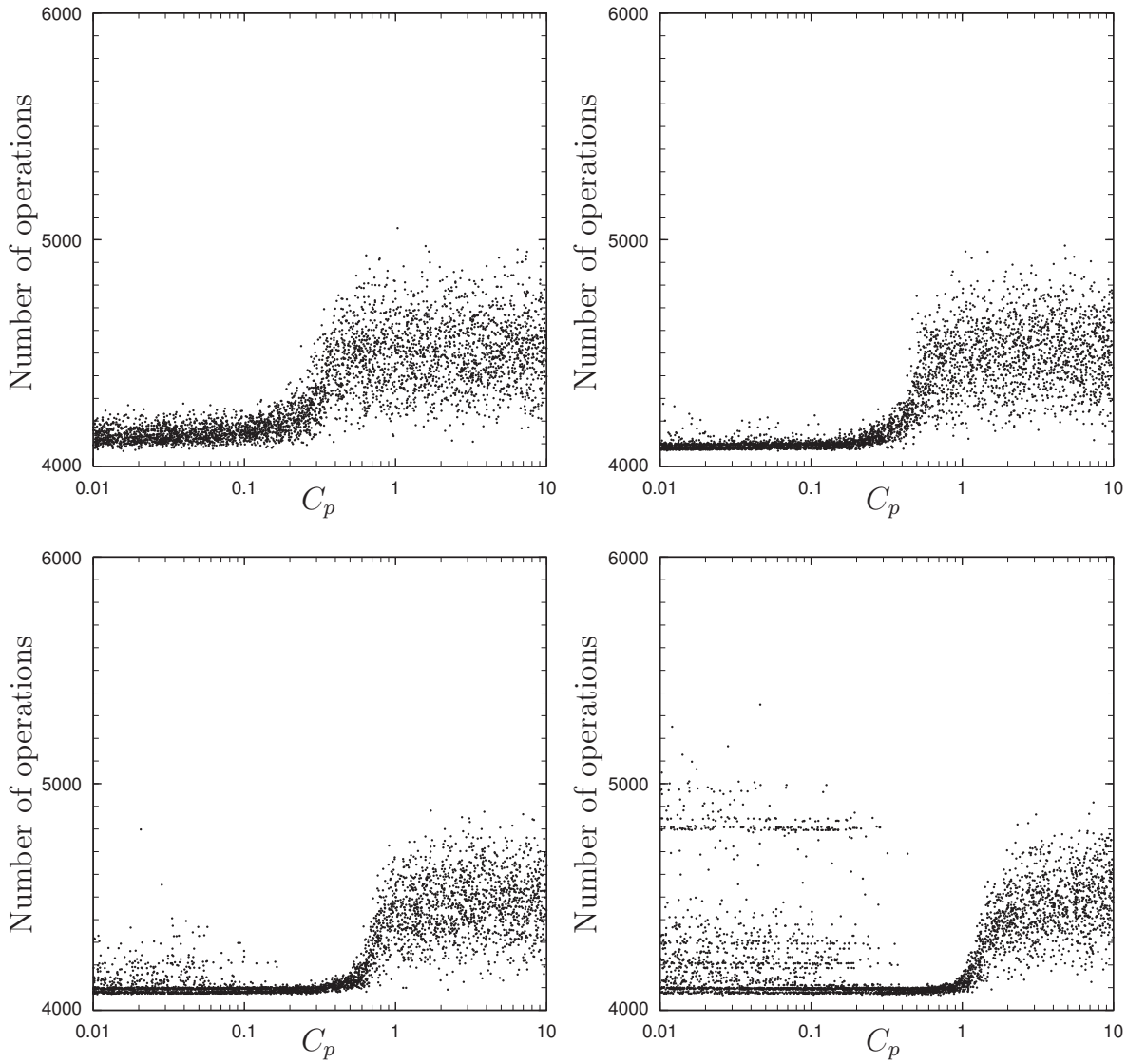

Figure 9: The physics formula HEP(σ) with 30 runs of 100 expansions, 18 runs of 167 expansions, 10 runs of 300 expansions and 3 runs of 1000 expansions respectively. The plot with one run of 3000 expansions can be found in Fig. 5, left bottom.

a shift of variables. This could work in a large number of cases. Such a shift would be one of the types

$$x_i \rightarrow x_i + a x_j \tag{10}$$

$$x_i \rightarrow x_i + a. \tag{11}$$

With such a shift the number of variables remains the same and hence the work for the optimizer (the size of the tree) does not become more complicated. This work can in principle be done in a generic procedure of about 100 lines. We have opted for a more sophisticated method that takes into account that there are various types of variables that only mix amoung each other. This would be the case when variables have different dimensions. The procedures

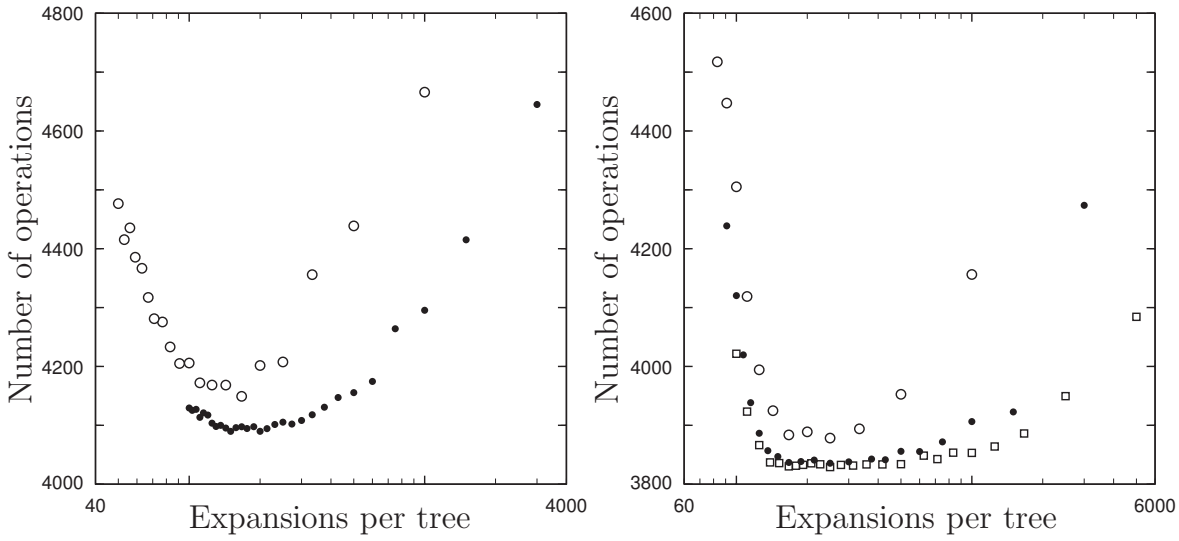

Figure 10: Number of operations as a function of the number of tree expansions per tree. The product of the number of expansions and the number of runs is kept constant (1000 for the open dots, 3000 for the filled dots and 5000 for the open squares). The dots are average results obtained by running the program 50 times. The left graph is for the HEP(σ) formula and the right graph is for the 7-4 resultant.

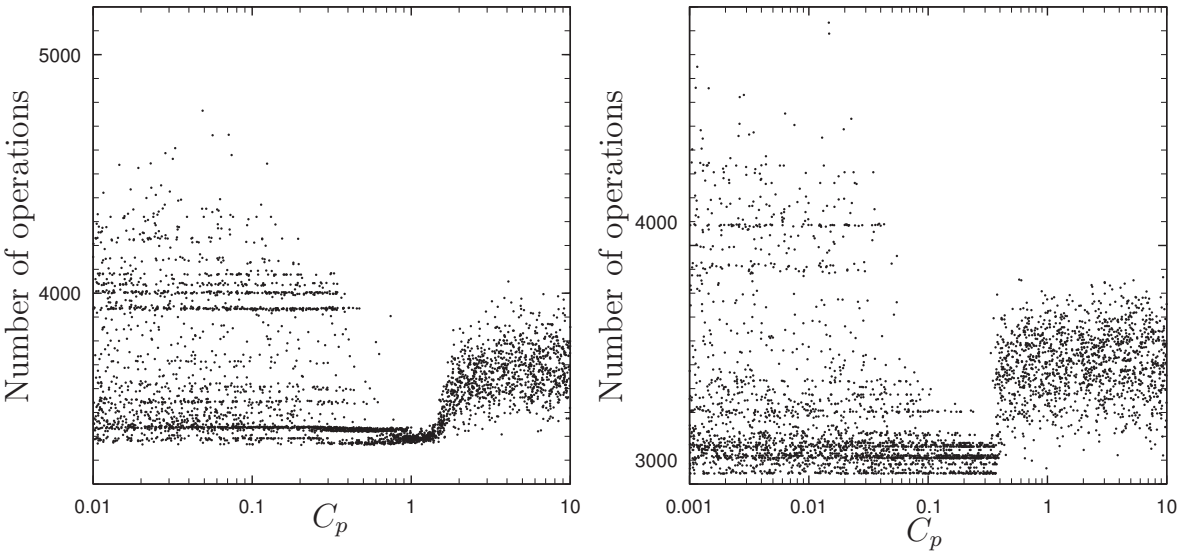

Figure 11: Each plot has 4000 runs. The runs include the greedy optimization. The left plot is the physics formula HEP(σ) with the backward direction and 3000 expansion per MCTS run, corresponding to Fig. 5 left bottom, and the right plot is the 7-4 resultant with the forward direction and 5000 expansion per MCTS run, corresponding to Fig. 7.

are included with the other files (doshift.hh) that contain the examples of this paper. The procedures look for potential replacements and if they make the expression shorter (= fewer terms) the new expression replaces the old one. It keeps doing this until all potential improvements are exhausted. In principle one could do this until a given number of attempts

has been made (the algorithm is basically quadratic in the number of terms) because the final improvements are usually rather small.

The shift procedure does not work for the resultants. The reason is that it looks for combinations like $\cdots(a_i x_i + a_j x_j + \cdots)$ with x_i and x_j not occurring outside the brackets, and then it tries the substitution $x_i \to x_i - a_j x_j / a_j$. Such combinations do not occur in the resultants. On the other hand in the physics formulas the results are very favorable. It is however important to notice that the order of declaration of the variables is important and hence one may have to experiment a little bit with this. For the three formulas we treat here some general rules could be set up.

The Feynman parameters were treated in a special way. In the end we want to bracket in them. Hence at first one might think that we should not be shifting them. If however we shift them too (but just combining Feynman parameters with each other or numbers) we obtain much better results. At the end we have to add some code to 'unshift' the Feynman parameters, so that in the original parameters the code becomes a bit lengthier again. Also this can be optimized, although it is a bit rough on the MCTS method because now there are many different variables (the coefficients of the shifted brackets). In the Tab. 6 we present the full results. If there are two numbers the numbers refer to the number of operations after the optimization plus the number of operations in the shift. When there are three numbers they represent the number of operations after the main optimization, the number of operations in the unshifting of the Feynman parameters and the number of operations in the shifts themselves.

	HEP(σ)	HEP(σ)	F_{13}	F_{24}
Variables	15	4+11	5+24	5+31
Expressions	1	35	56	56
Terms	5 717	5 717	105 114	836 010
Format O0	47 424	33 798	812 645	5 753 030
Format O1	6 099	5 615	71 989	391 663
Format O2	4 979	4 599	46 483	233 445
Format O3	3 423	3 380	41 666	195 691
Terms shifted	754	754	16 439	78 005
Format O0	6 278+29	4 402+731+15	123 415+605+48	536 127+476+57
Format O1	1 549+29	1 481+409+15	23 459+453+48	68 093+336+57
Format O2	1 216+29	1 146+261+15	17 620+330+48	53 131+229+57
Format O3	976+29	1 012+261+15	13 206+322+48	47 379+235+57

Table 6: Results for the physics formulas in the original and the shifted versions. The counting of the number of operations takes the brackets in the Feynman parameters into account unlike ref [4]. When the number of variables is presented as a sum, the first number is the number of Feynman parameters and we do simultaneous optimizations.

The improvements are significant and in addition the FORM optimization runs become faster because their input expressions are shorter. Also the compile times go down considerably. The reason that this shifting works so well is that effectively it selects simple popular common subexpressions and expresses the formula in terms of these. This makes that the Horner scheme will be affected and so will the optimizations after it.

Of course other types of problems may benefit from other approaches. If one is resigned

to not try the O3 option, the number of variables may be less of an obstacle and one may try 'partial replacements'. These act on only a fraction of the terms. Such replacements cause the number of variables to increase. The structure of the formulas will dictate what to try and how to try it. This is what we call domain specific and it falls outside the scope of this paper.

7 Conclusions and outlook

The inclusion of adaptable Horner schemes, the common subexpressions and the greedy optimizations add considerable power to the flexibility of the FORM output and make it competitive, if not better, than all systems we could compare it with. The additional MCTS methods improve the optimizations even further, although this goes at the cost of computer resources. Because the method is completely new for this field, it is not yet known how the various parameters should be tuned to the formulas that are optimized. The section on the selection of the parameters should aid the user in determining experimentally what is optimal for the problems at hand. If the computer time invested in these experiments is relatively unimportant, the payoff can be large. In particular the tuning of the UCT parameter C_p and the selection of the direction of the tree search through the relevant variables are important and can make much difference in the final result. The use of several trees each with a smaller number of expansions can also have a great influence. We hope to be able to implement ways to automatically determine these parameters in future versions of FORM.

Additional methods that would for instance recognize subexpressions that are powers of simpler composite objects are much harder to implement. Currently they have not been developed to a level that allows implementation. Therefore we encourage users to consider these 'domain specific' and look for such simplifications in their programs. Often knowledge about the problem allows one to find a number of them.

The examples we used can be found in the FORM site (http://www.nikhef.nl/∼form)

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