

Symbolic Programming by Example

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<http://wwwth.mpp.mpg.de/members/hahn/sym.pdf>

<http://wwwth.mpp.mpg.de/members/hahn/sym.tar.gz>



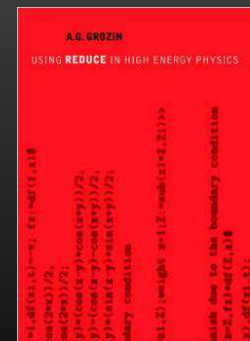
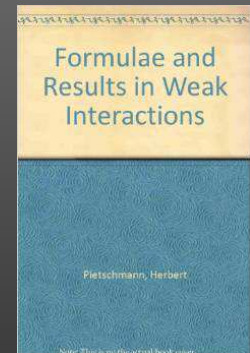
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Reference Books, Formula Collections

- V.I. Borodulin et al.
CORE (Compendium of Relations)
arXiv:1702.08246.
- Herbert Pietschmann
Formulae and Results in Weak Interactions
Springer (Austria) 2nd ed., 1983.
- Andrei Grozin
Using REDUCE in High-Energy Physics
Cambridge University Press, 1997.



Antisymmetric Tensor

The **Antisymmetric Tensor in n dimensions** is denoted by $\varepsilon_{i_1 i_2 \dots i_n}$. You can think of it as a matrix-like object which has either -1 , 0 , or 1 at each position.

For example, the **Determinant** of a matrix, being a **completely antisymmetric** object, can be written with the ε -tensor:

$$\det A = \sum_{i_1, \dots, i_n=1}^n \varepsilon_{i_1 i_2 \dots i_n} A_{i_1 1} A_{i_2 2} \cdots A_{i_n n}$$

In practice, the ε -tensor is usually contracted, e.g. with vectors. We will adopt the following notation to avoid dummy indices:

$$\varepsilon_{\mu\nu\rho\sigma} p^\mu q^\nu r^\rho s^\sigma = \varepsilon(p, q, r, s).$$



Antisymmetric Tensor in Mathematica

```
Eps[___, p_, ___, p_, ___] := 0
```

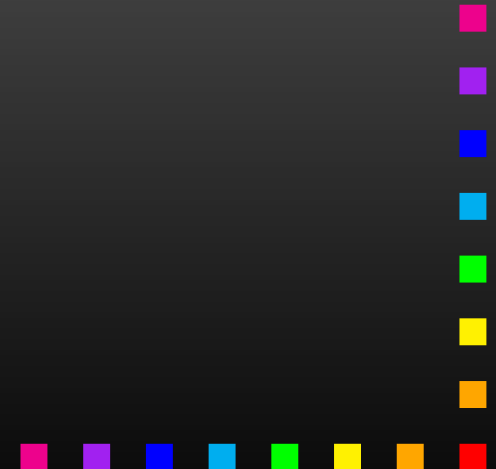
```
(* implement linearity: *)
```

```
Eps[a___, p_Plus, b___] := Eps[a, #, b]&/@ p
```

```
Eps[a___, n_?NumberQ r_, b___] := n Eps[a, r, b]
```

```
(* otherwise sort the arguments into canonical order: *)
```

```
Eps[args__] := Signature[{args}] Eps@@ Sort[{args}] /;  
!OrderedQ[{args}]
```



Momentum Conservation

Problem: **Proliferation of terms** in expressions such as

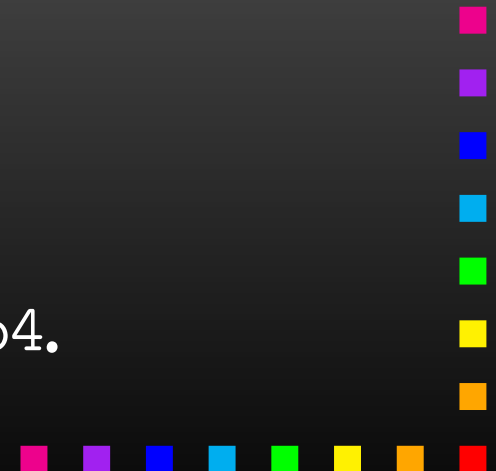
$$\begin{aligned}d &= \frac{1}{(p_1 + p_2 - p_3)^2 + m^2} \\ &= \frac{1}{p_1^2 + p_2^2 + p_3^2 + 2p_1p_2 - 2p_2p_3 - 2p_1p_3 + m^2}'\end{aligned}$$

whereas if $p_1 + p_2 = p_3 + p_4$ we could have instead

$$d = \frac{1}{p_4^2 + m^2}.$$

In Mathematica: just do $d /. p1 + p2 - p3 -> p4$.

Problem: FORM cannot replace sums.



Momentum Conservation in FORM

Idea: for each expression x , add and subtract a zero, i.e. form

$\{x, y = x + 0, z = x - 0\}$, where e.g. $0 = p_1 + p_2 - p_3 - p_4$,

then select the shortest expression. But: how to select the shortest expression (in FORM)?

Solution: add the number of terms of each argument, i.e.

$$\{x, y, z\} \rightarrow \{x, y, z, n_x, n_y, n_z\}.$$

Then sort n_x, n_y, n_z , but when exchanging n_a and n_b ,
exchange also a and b :

```
symm 'foo' (4,1) (5,2) (6,3);
```

This unconventional sort statement is rather typical for FORM.

Momentum Conservation in FORM

```
#procedure Shortest(foo)

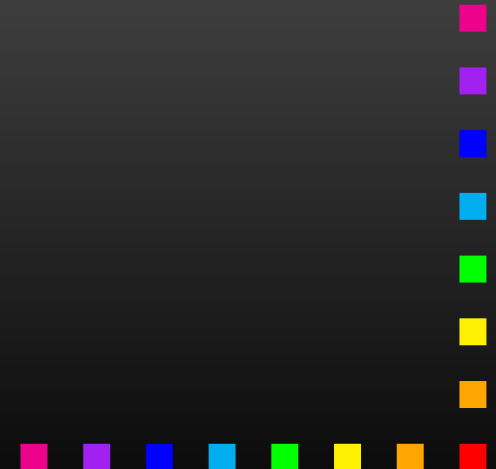
id 'foo'([x]?) = 'foo'([x], [x] + 'MomSum', [x] - 'MomSum');

* add number-of-terms arguments
id 'foo'([x]?, [y]?, [z]?) = 'foo'([x], [y], [z],
  nterms_([x]), nterms_([y]), nterms_([z]) );

* order according to the nterms
symm 'foo' (4,1) (5,2) (6,3);

* choose shortest argument
id 'foo'([x]?, ?a) = 'foo'([x]);

#endprocedure
```



Abbreviationing

One of the most powerful tricks to both **reduce the size** of an expression and **reveal its structure** is to substitute subexpressions by new variables.

The essential function here is `Unique` with which new symbols are introduced. For example,

```
Unique["test"]
```

generates e.g. the symbol `test1`, which is **guaranteed not to be in use so far**.

The `Module` function which implements lexical scoping in fact uses `Unique` to rename the symbols internally because **Mathematica can really do dynamical scoping only**.



Abbreviating in Mathematica

```
$AbbrPrefix = "c"
```

```
abbr[expr_] := abbr[expr] = Unique[$AbbrPrefix]
```

```
(* abbreviate function *)
```

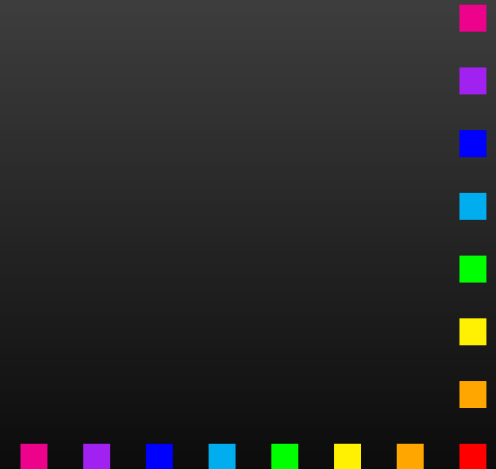
```
Structure[expr_, x_] := Collect[expr, x, abbr]
```

```
(* get list of abbreviations *)
```

```
AbbrList[] := Cases[DownValues[abbr],  
  _[_[_[f_]], s_Symbol] -> s -> f]
```

```
(* restore full expression *)
```

```
Restore[expr_] := expr /. AbbrList[]
```



Abbreviation in FORM

* collect w.r.t. some function

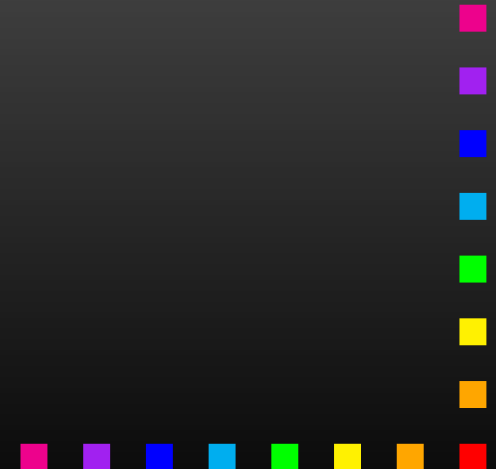
```
b Den;  
.sort  
collect acc;
```

* introduce abbreviations for prefactors

```
toPolynomial onlyfunctions acc;  
.sort
```

* print abbreviations & abbreviated expr

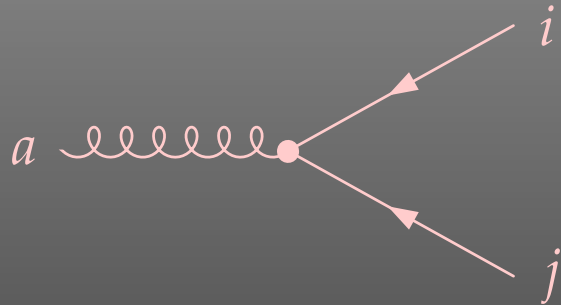
```
#write "%X"  
print +s;
```



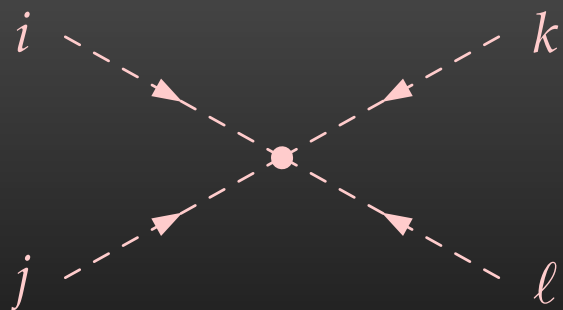
Color Structures

In Feynman diagrams four types of **Color structures** appear:

Natural Representation

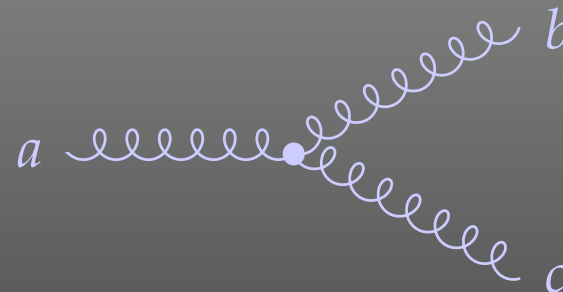


$$\sim T_{ij}^a = \text{SUNT}[a, i, j]$$

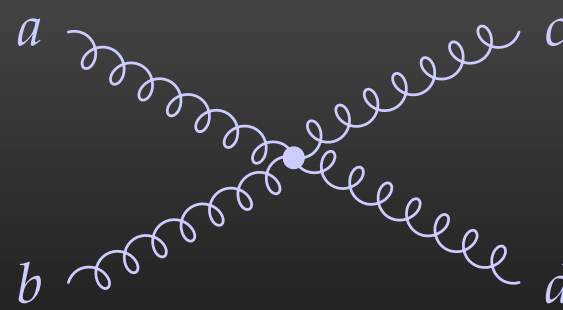


$$\sim T_{ij}^a T_{kl}^a = \text{SUNTSum}[i, j, k, l]$$

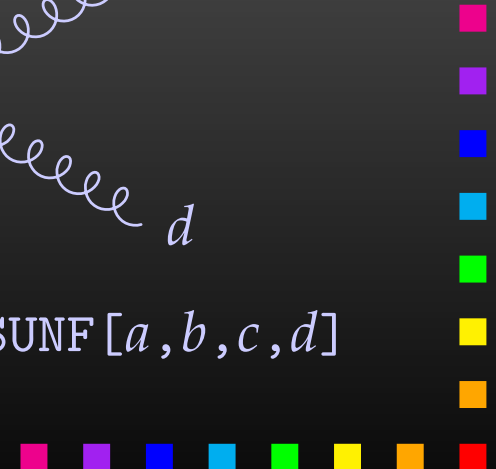
Adjoint Representation



$$\sim f^{abc} = \text{SUNF}[a, b, c]$$



$$\sim f^{abx} f^{xcd} = \text{SUNF}[a, b, c, d]$$



Unified Notation

The SUNF's can be converted to SUNT's via

$$f^{abc} = 2i [\text{Tr}(T^c T^b T^a) - \text{Tr}(T^a T^b T^c)].$$

We can now represent all color objects by just SUNT:

- $\text{SUNT}[i, j] = \delta_{ij}$
- $\text{SUNT}[a, b, \dots, i, j] = (T^a T^b \dots)_{ij}$
- $\text{SUNT}[a, b, \dots, 0, 0] = \text{Tr}(T^a T^b \dots)$

This notation again avoids **unnecessary dummy indices**.
(Mainly namespace problem.)

For purposes such as the “large- N_c limit” people like to use **SU(N)** rather than an explicit **SU(3)**.



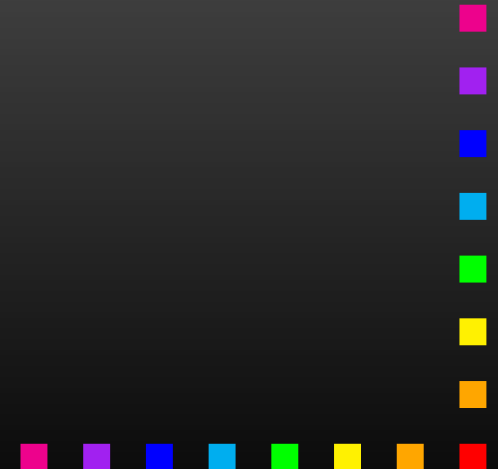
Fierz Identities

The **Fierz Identities** relate expressions with **different orderings of external particles**. The Fierz identities essentially express completeness of the underlying matrix space.

They were originally found by Markus Fierz in the context of Dirac spinors, but can be generalized to any finite-dimensional matrix space [hep-ph/0412245].

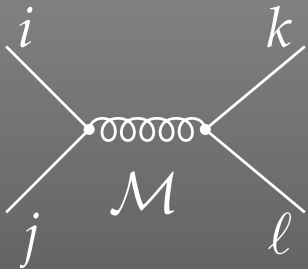
For SU(N) (color) reordering, we need

$$T_{ij}^a T_{kl}^a = \frac{1}{2} \left(\delta_{il} \delta_{kj} - \frac{1}{N} \delta_{ij} \delta_{kl} \right).$$



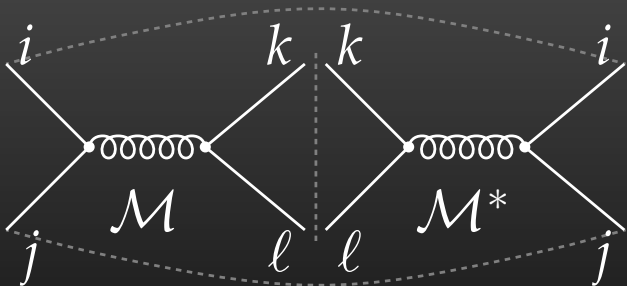
Cvitanovich Algorithm

For an **Amplitude**:



- convert all color structures to (generalized) SUNT objects,
- simplify: apply Fierz identity on all internal gluon lines,
- expect SUNT with indices of external particles to remain.

For a **Squared Amplitude**:



- use the Fierz identity to get rid of all SUNT objects,
- expect SUNT to vanish, color factors (numbers) only.

For “hand” calculations, a pictorial version of this algorithm exists in the literature.



Color Simplify in FORM

* introduce dummy indices for the traces

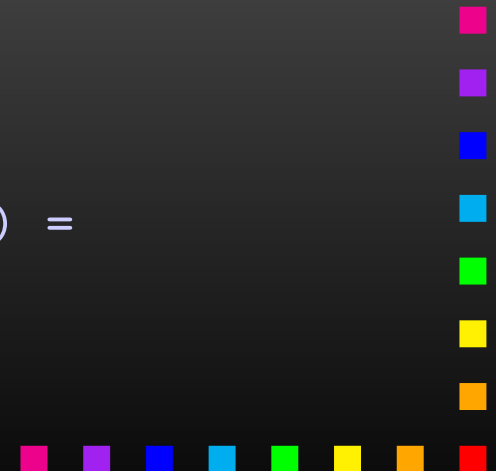
```
repeat;  
  once SUNT(?a, 0, 0) = SUNT(?a, DUMMY, DUMMY);  
  sum DUMMY;  
endrepeat;
```

* take apart SUNTs with more than one T

```
repeat;  
  once SUNT(?a, [a]?, [b]?, [i]?, [j]?) =  
    SUNT(?a, [a], [i], DUMMY) * SUNT([b], DUMMY, [j]);  
  sum DUMMY;  
endrepeat;
```

* apply the Fierz identity

```
id SUNT([a]?, [i]?, [j]?) * SUNT([a]?, [k]?, [l]?) =  
  1/2 * SUNT([i], [l]) * SUNT([j], [k]) -  
  1/2/('SUNN') * SUNT([i], [j]) * SUNT([k], [l]);
```



Translation to Color-Chain Notation

In color-chain notation we can distinguish two cases:

a) Contraction of **different chains**:

$$\langle A | T^a | B \rangle \langle C | T^a | D \rangle = \frac{1}{2} \left(\langle A | D \rangle \langle C | B \rangle - \frac{1}{N} \langle A | B \rangle \langle C | D \rangle \right),$$

b) Contraction on the **same chain**:

$$\langle A | T^a | B | T^a | C \rangle = \frac{1}{2} \left(\langle A | C \rangle \text{Tr } B - \frac{1}{N} \langle A | B | C \rangle \right).$$



Color Simplify in Mathematica

```
(* same-chain version *)
```

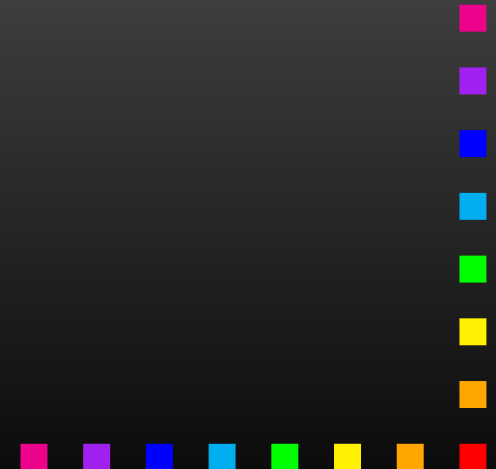
```
sunT[t1___, a_Symbol, t2___, a_, t3___, i_, j_] :=  
  (sunT[t1, t3, i, j] sunTrace[t2] -  
   sunT[t1, t2, t3, i, j]/SUNN)/2
```

```
(* different-chain version *)
```

```
sunT[t1___, a_Symbol, t2___, i_, j_] *  
sunT[t3___, a_, t4___, k_, l_] ^:=  
  (sunT[t1, t4, i, l] sunT[t3, t2, k, j] -  
   sunT[t1, t2, i, j] sunT[t3, t4, k, l]/SUNN)/2
```

```
(* introduce dummy indices for the traces *)
```

```
sunTrace[a__] := sunT[a, #, #]&[ Unique["col"] ]
```



Fermion Trace

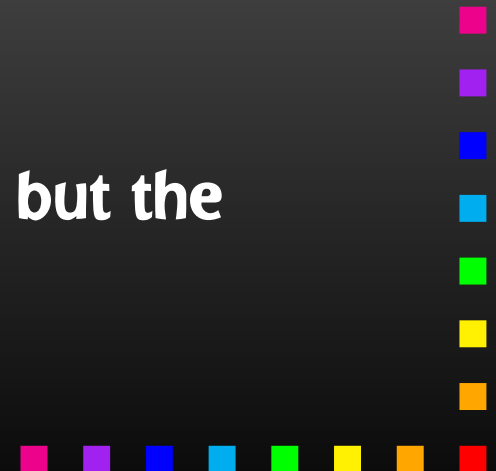
Leaving apart problems due to γ_5 in d dimensions, we have as the main algorithm for the 4d case:

$$\begin{aligned}\text{Tr } \gamma_\mu \gamma_\nu \gamma_\rho \gamma_\sigma \cdots &= + g_{\mu\nu} \text{Tr } \gamma_\rho \gamma_\sigma \cdots \\ &\quad - g_{\mu\rho} \text{Tr } \gamma_\nu \gamma_\sigma \cdots \\ &\quad + g_{\mu\sigma} \text{Tr } \gamma_\nu \gamma_\rho \cdots\end{aligned}$$

This algorithm is recursive in nature, and we are ultimately left with

$$\text{Tr } \mathbb{1} = 4.$$

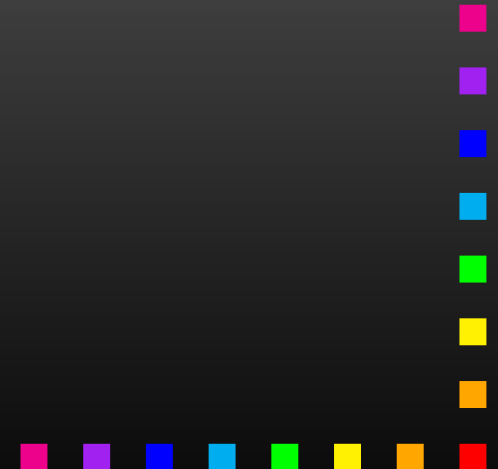
(Note that this 4 is not the space-time dimension, but the dimension of spinor space.)



Fermion Trace in Mathematica

```
Trace4[mu_, g__] :=  
Block[ {Trace4, s = -1},  
  Plus@@ MapIndexed[  
    ((s = -s) Pair[mu, #1] Drop[Trace4[g], #2])&,  
    {g} ]  
]
```

```
Trace4[] = 4
```



Tensor Reduction

The loop integrals corresponding to closed loops in a Feynman integral in general have a **tensor structure** due to **integration momenta in the numerator**. For example,

$$B_{\mu\nu}(p) = \int d^d q \frac{q_\mu q_\nu}{(q^2 - m_1^2) ((q - p)^2 - m_2^2)}.$$

Such tensorial integrals are rather unwieldy in practice, therefore they are reduced to linear combinations of Lorentz-covariant tensors, e.g.

$$B_{\mu\nu}(p) = B_{00}(p) g_{\mu\nu} + B_{11}(p) p_\mu p_\nu.$$

It is the **coefficient functions** B_{00} and B_{11} which are implemented in a library like LoopTools.



Tensor Reduction Algorithm

The first step is to **convert the integration momenta** in the numerator to an actual tensor, e.g. $q_\mu q_\nu \rightarrow N_{\mu\nu}$. FORM has the special command `totensor` for this:

```
totensor q1, NUM;
```

The next step is to **take out $g_{\mu\nu}$'s in all possible ways**. We do this in form of a sum:

$$N_{\mu_1 \dots \mu_n} = \sum_{i=0,2,4,\dots}^n \pi(0)^i \sum_{\substack{\text{all } \{\nu_1, \dots, \nu_i\} \\ \in \{\mu_1, \dots, \mu_n\}}} g_{\nu_1 \nu_2} \cdots g_{\nu_{i-1} \nu_i} N_{\mu_1 \dots \mu_n \setminus \nu_1 \dots \nu_i}$$

The $\pi(0)^i$ **keeps track of the indices** of the tensor coefficients, i.e. it later provides the two zeros for every $g_{\mu\nu}$ in the index, as in D_{0012} .



Tensor Reduction Algorithm

To fill in the remaining $\pi(i)$'s, we start off by **tagging the arguments** of the loop function, which are just the momenta. For example:

$$C(p_1, p_2, \dots) \rightarrow \tau(\pi(1)p_1 + \pi(2)p_2) C(p_1, p_2, \dots)$$

The temporary function τ keeps its argument, the 'tagged' momentum p , separate from the rest of the amplitude.

Now **add the indices** of $N_{\mu_1 \dots \mu_n}$ to the momentum in τ :

$$\tau(p) N_{\mu_1 \dots \mu_n} = p_{\mu_1} \cdots p_{\mu_n}.$$

Finally, collect all π 's into the tensor-coefficient index.



Tensor Reduction in FORM

```
totensor q1, NUM;
```

```
* take out 0, 2, 4... indices for g_{mu nu}
```

```
id NUM(?b) = sum_(DUMMY, 0, nargs_(?b), 2,  
  pave(0)^DUMMY * distrib_(1, DUMMY, dd_, NUM, ?b));
```

```
* construct tagged momentum in TMP
```

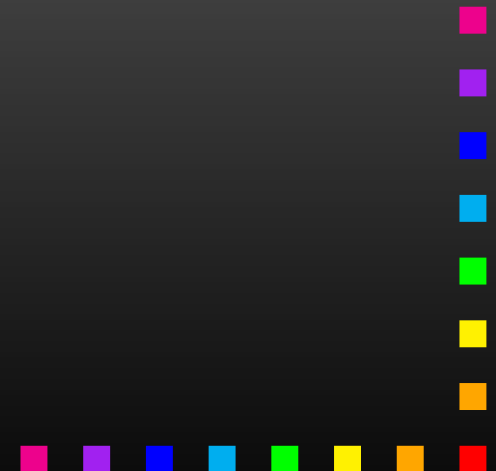
```
id COi([p1]?, [p2]?, ?a) = TMP(pave(1)*[p1] + pave(2)*[p2]) *  
  COi(MOM([p1]), MOM([p2] - [p1]), MOM([p2]), ?a);
```

```
* expand momentum
```

```
repeat id TMP([p1]?) * NUM([mu]?, ?a) =  
  d_([p1], [mu]) * NUM(?a) * TMP([p1]);
```

```
* collect the indices
```

```
chainin pave;
```

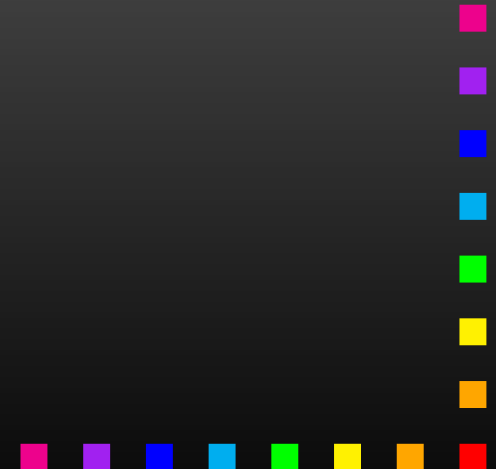


Tensor Reduction in Mathematica

```
tens[i_, p_][mu_, nu___] :=  
Block[ {tens},  
    (* take out g *)  
    { MapIndexed[g[mu, #1] Drop[tens[{i,0,0}, p][nu], #2]&, {nu}],  
      (* take out p *)  
      (#1[mu] tens[{i,#2}, p][nu])&@@@ p }  
]
```

```
tens[i_, _][] := C@@ Sort[Flatten[i]]
```

```
FindTensors[mu_, p_] :=  
Block[ {tenslist},  
    tenslist = tens[{}], MapIndexed[List, p]]@@ mu;  
    Collect[Plus@@ Flatten[tenslist], _C]  
]
```



More Complex Calculations

Often special requirements:

- **Resummations** (e.g. *hbb* in MSSM),
- **Approximations** (e.g. gaugeless limit),
- **K-factors**,
- **Nontrivial renormalization.**

Software design so far:

- Mostly '**monolithic**' (one package does everything).
- Often controlled by **parameter cards**, not easy to use beyond intended purpose.
- May want to/must use other packages.



Example: $\mathcal{O}(\alpha_t^2)$ MSSM Higgs-mass corrections

Hollik, Paßehr 2014

Shopping List for the Diagrammatic Calculation:

① Unrenormalized 2L self-energies

$$\Sigma_{hh}^{(2)}, \Sigma_{hH}^{(2)}, \Sigma_{hA}^{(2)}, \Sigma_{HH}^{(2)}, \Sigma_{HA}^{(2)}, \Sigma_{AA}^{(2)}, \Sigma_{H^+H^-}^{(2)}$$

in gaugeless approximation at $p^2 = 0$ at $\mathcal{O}(\alpha_t^2)$.

② 1L diagrams with insertions of 1L counterterms.

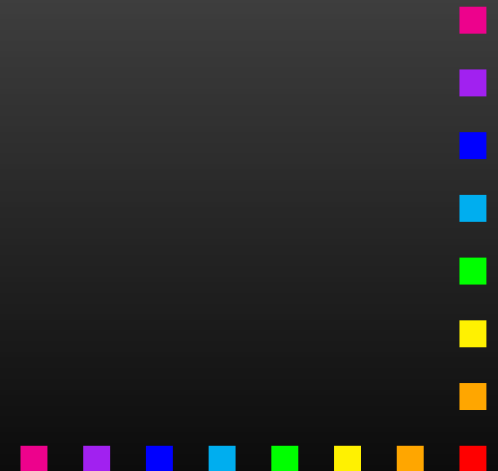
③ 2L counterterms for ①.

④ 2L tadpoles $T_h^{(2)}, T_H^{(2)}, T_A^{(2)}$ at $\mathcal{O}(\alpha_t^2)$ appearing in ③.



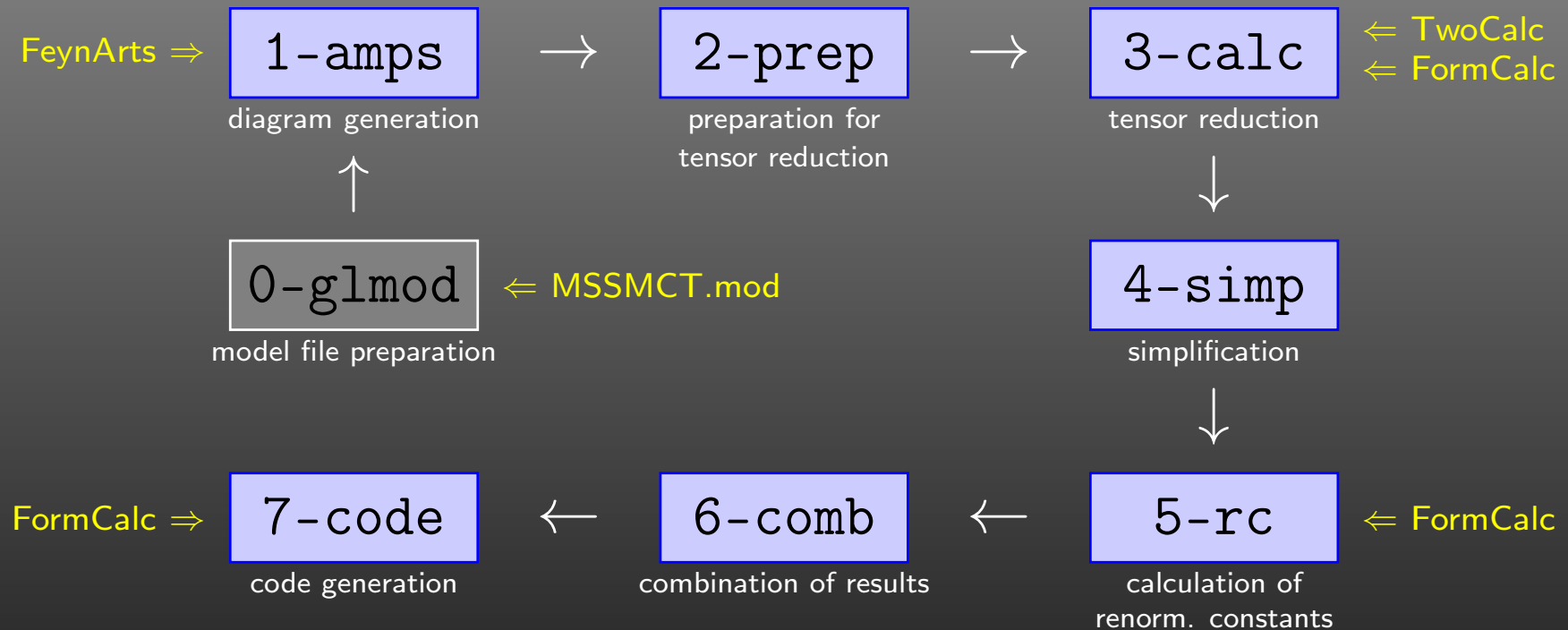
Template for Calculations

- Break calculation into **several steps**.
- Implement each step as **independent program** (invoked from command line).
- In lieu of 'in vivo' debugging **keep detailed logs**.
- Coordinate everything through a **makefile**.



Steps of the Calculation

Calculation split into 7 (8) steps:



Script Structure

- **Shell scripts** (`/bin/sh`), run from command line as e.g.
`./1-amps arg1 arg2`
- `arg1` = `h0h0`, `h0HH`, `h0A0`, `HHHH`, `HHA0`, `A0A0`, `HmHp` (**self-energies**),
`h0`, `HH`, `A0` (**tadpoles**).
- `arg2` = `0` for virtual 2L diagrams,
`1` for 1L diagrams with 1L counterterms.

- **Inputs/outputs defined in first few lines, e.g.**

```
in=m/$1/2-prep.$2  
out=m/$1/3-calc.$2
```

- **Symbolic output + log files go to 'm' subdirectory.**
Log file = Output file + .log.gz
- **Fortran code goes to 'f' subdirectory.**



Step 0: Gaugeless Limit

Gaugeless approximation:

- ① Set gauge couplings $g, g' = 0 \Rightarrow M_W, M_Z = 0$.
- ② Keep finite weak mixing angle.
- ③ Keep $\frac{\delta M_W^2}{M_W^2}$ and $\frac{\delta M_Z^2}{M_Z^2}$ finite.

Must set $m_b = 0$ so that $\mathcal{O}(\alpha_t^2)$ corrections form supersymmetric and gauge-invariant subset.

Most efficient to **modify Feynman rules** (not ③, though):

- Load MSSMCT.mod model file.
- Modify couplings, remove zero ones.
- Write out MSSMCTg1.mod model file.



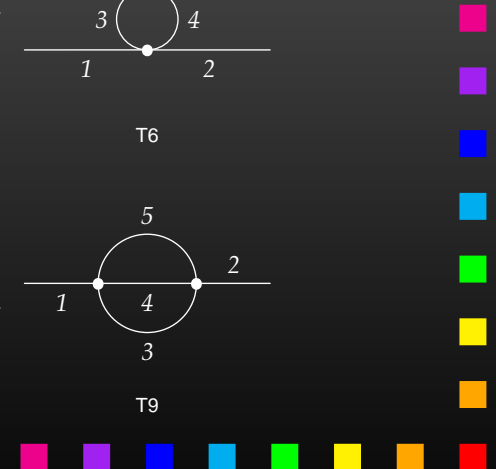
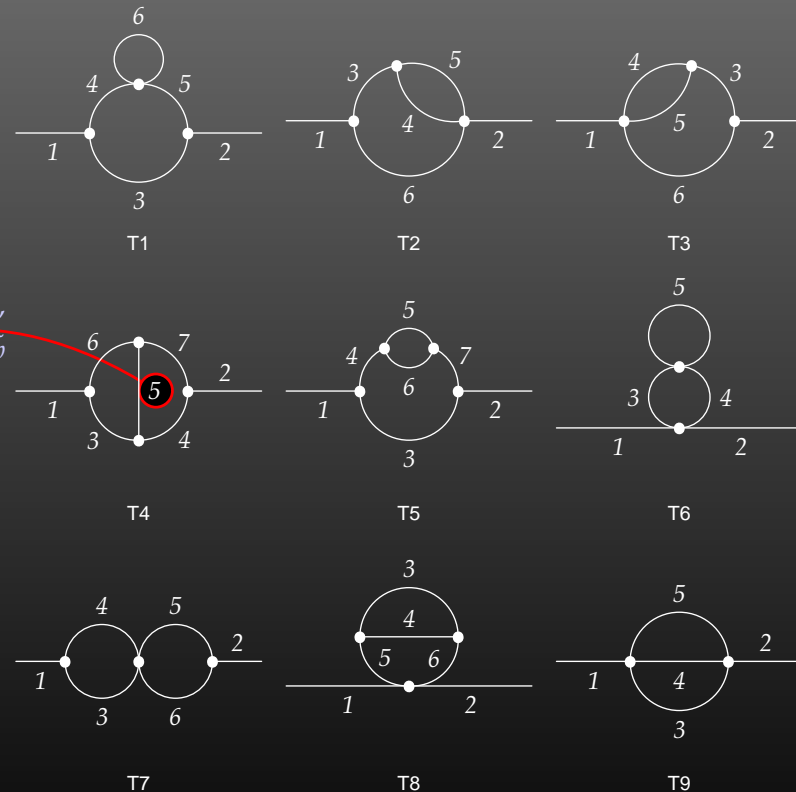
Step 1: Diagram Generation

- Generate 2L virtual and 1L+counterterm diagrams using wrappers for FeynArts functions.

Simple diagram selection functions, e.g.

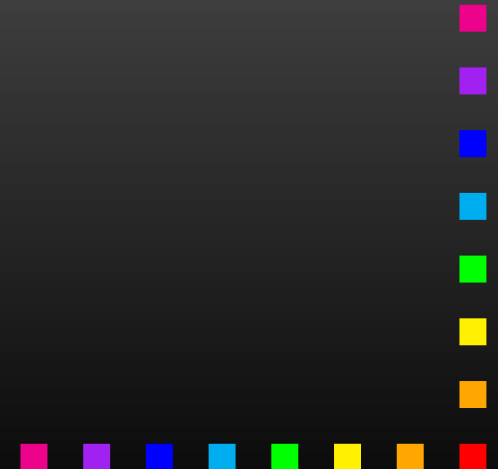
```

sel[0][S[_] -> S[_]] = {
  t[3] && htb[6],
  t[3] && tb[6],
  t[3] && tb[6],
  t[3] && t[4] && htb[5],
  t[3] && htb[5|6],
  t[3] && htb[5],
  t[3] && t[5],
  t[5] && ht[3|4],
  t[3|4|5] && ht[3|4|5] }
  
```



Step 2: Preparation for Tensor Reduction

- Take $p^2 \rightarrow 0$ limit.
- Simplify ubiquitous sfermion mixing matrices U_{ij} , mostly by exploiting unitarity ($\sim 50\%$ size reduction).



Efficiently Exploit Unitarity in Mathematica

Unitarity of 2 x 2 matrix: $UU^\dagger = U^\dagger U = \mathbb{1}$, i.e.

$$U_{11}U_{11}^* + U_{12}U_{12}^* = 1, \quad U_{11}U_{21}^* + U_{12}U_{22}^* = 0,$$

$$U_{21}U_{21}^* + U_{22}U_{22}^* = 1, \quad U_{21}U_{11}^* + U_{22}U_{12}^* = 0,$$

$$U_{11}U_{11}^* + U_{21}U_{21}^* = 1, \quad U_{11}U_{12}^* + U_{21}U_{22}^* = 0,$$

$$U_{12}U_{12}^* + U_{22}U_{22}^* = 1, \quad U_{12}U_{11}^* + U_{22}U_{21}^* = 0.$$

Problem: Simplify will **rarely arrange the U 's in just the way** that these rules can be applied directly.

Solution: Introduce auxiliary symbols which **immediately deliver** the r.h.s. once Simplify considers the l.h.s., i.e. **increase the 'incentive'** for Simplify to use the r.h.s.

But: Upvalues work only one level deep.



Efficiently Exploit Unitarity in Mathematica

Introduce

$$USf[1, j] USfC[1, j] \rightarrow UCSf[1, j],$$

$$USf[2, j] USfC[2, j] \rightarrow UCSf[2, j],$$

$$USf[1, j] USfC[2, j] \rightarrow UCSf[3, j], \quad + \text{ ditto for 1}^{\text{st}} \text{ index}$$

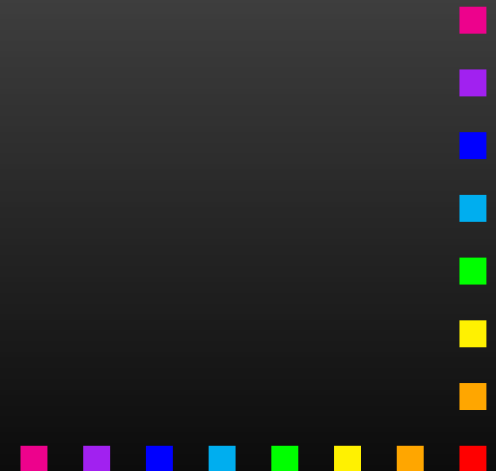
and formulate unitarity for the UCSf:

$$\begin{aligned} UCSf[2, 1] &= UCSf[1, 2]; & UCSf[3, 2] &= -UCSf[3, 1]; \\ UCSf[2, 2] &= UCSf[1, 1]; & UCSfC[3, 2] &= -UCSfC[3, 1]; \\ & & UCSf[2, 3] &= -UCSf[1, 3]; \\ \dots & & UCSfC[2, 3] &= -UCSfC[1, 3]; \end{aligned}$$



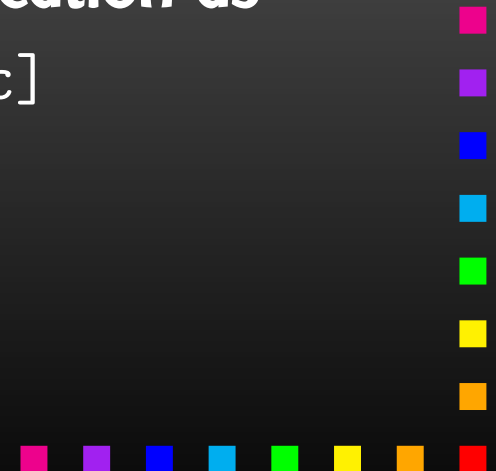
Step 3: Tensor Reduction

- Relatively straightforward application of **TwoCalc** and **FormCalc** for tensor reduction.
- Observe: Need **two Mathematica sessions** since TwoCalc and FormCalc cannot be loaded into one session, easily accomodated in shell script.



Step 4: Simplification

- Tensor reduction traditionally increases # of terms most.
- Step 4 reduces size before combination of results.
- Empirical simplification recipe.
- **'DiagMark' trick** (D. Stöckinger):
 - Introduce `DiagMark[mi]` where m_i = masses in loop in FeynArts output.
 - Few simplifications can be made between parts with different `DiagMark` \Rightarrow Can apply simplification as
`Collect[amp, _DiagMark, simpfunc]`
 - Much faster.



Step 5: Calculation of Renormalization Constants

- Compute 1L renormalization constants (RC) with FormCalc.

- Substitute explicit mass dependence in

$$dM_{Vsq1} \rightarrow MV2 dM_{Vsq1} MV2 \quad (V = W, Z)$$

such that gaugeless limit can be taken safely.

- Expand in ε , collect powers for easier handling later, e.g.

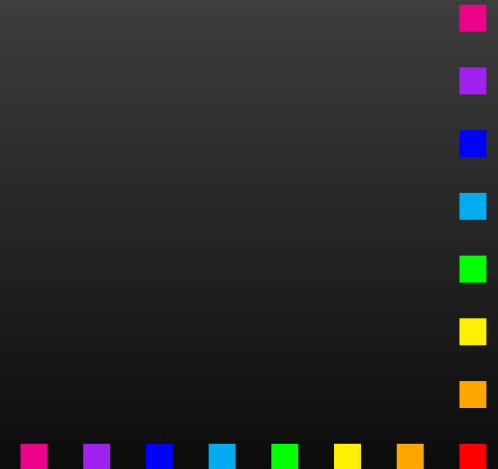
$$\left\{ \begin{array}{l} dM_{f1}[3,3] \rightarrow RC[-1, dM_{f1}[-1,3,3]] + \\ \quad \quad \quad RC[0, dM_{f1}[0,3,3]], \end{array} \right\} \text{ expansion}$$

$$\left\{ \begin{array}{l} dM_{f1}[-1,3,3] \rightarrow \dots, \\ dM_{f1}[0,3,3] \rightarrow \dots \end{array} \right\} \text{ actual expressions for } \varepsilon\text{-coeffs}$$



Step 6: Combination of Results

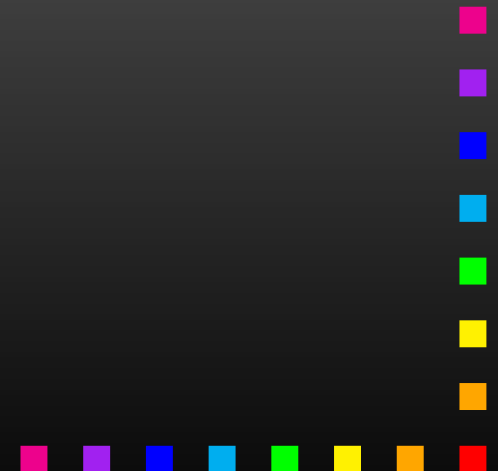
- Expand amplitude in ε (similar as RC).
- Insert RCs.
- Add genuine 2L counterterms (hand-coded).
- Pick only ε^0 term (unless debug flag set).
- Perform final simplification.



Step 7: Code Generation

- Introduce abbreviations to shorten code.
- Write out Fortran code using FormCalc's code-generation functions.
- Add static code which computes e.g. the necessary parameters for the generated code.
- Total final code size: 350 kBytes.

More details in [arXiv:1508.00562](https://arxiv.org/abs/1508.00562).



Exercise

Devise programs in Mathematica and FORM which apply the Dirac equation to a suitably defined spinor, i.e.

$$\not{p}_i |u_i\rangle = m_i |u_i\rangle$$

$$\not{p}_i |v_i\rangle = -m_i |v_i\rangle$$

<http://wwwth.mpp.mpg.de/members/hahn/sym.pdf>

<http://wwwth.mpp.mpg.de/members/hahn/sym.tar.gz>

