FeynArts and FormCalc in the era of the LHC

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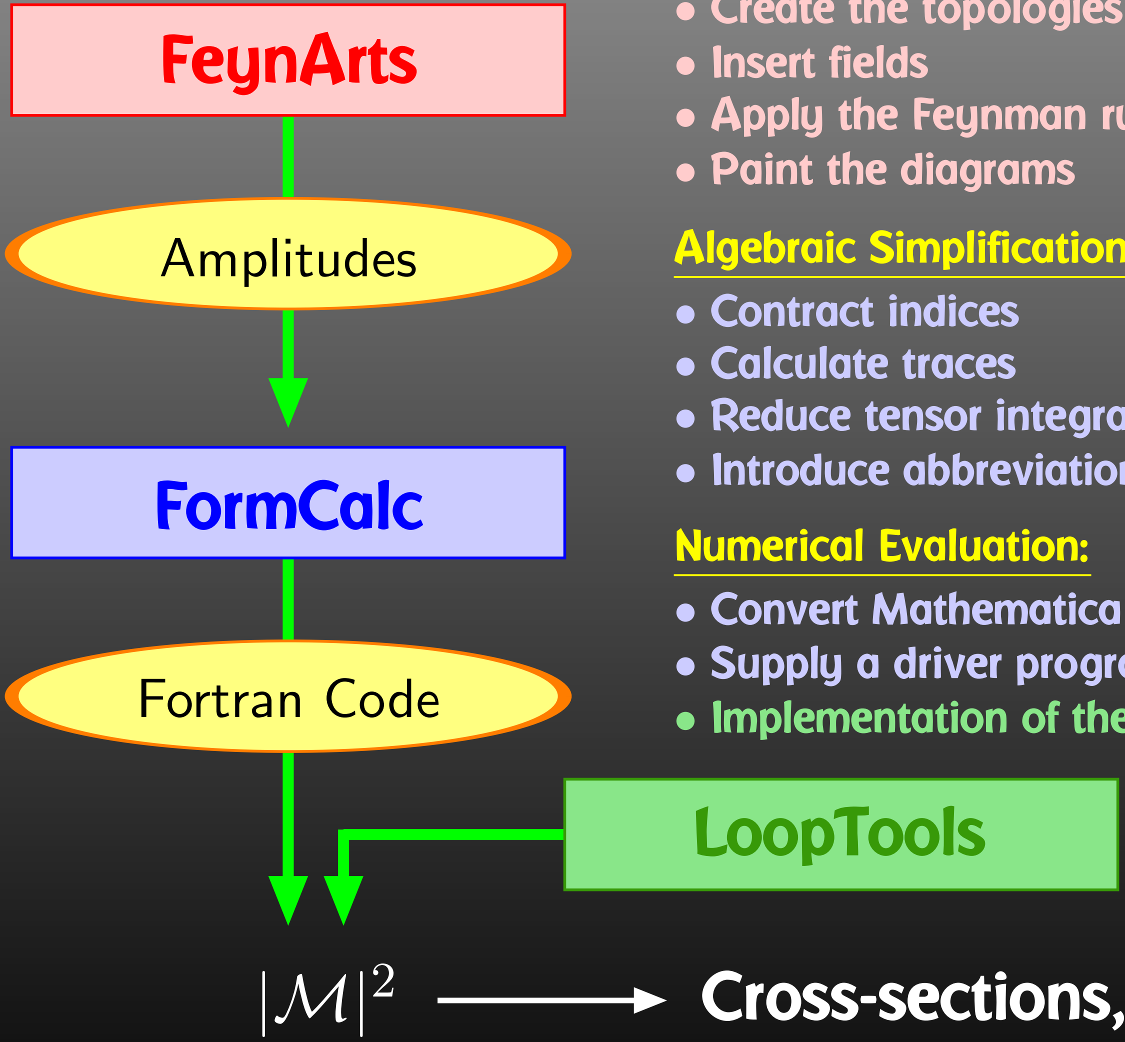
Automated Diagram Evaluation



$\longrightarrow$ **Cross-sections, Decay rates, . . .**

Diagram Generation:

- Create the topologies
- Insert fields
- Apply the Feynman rules
- Paint the diagrams

Algebraic Simplification:

- Contract indices
- Calculate traces
- Reduce tensor integrals
- Introduce abbreviations

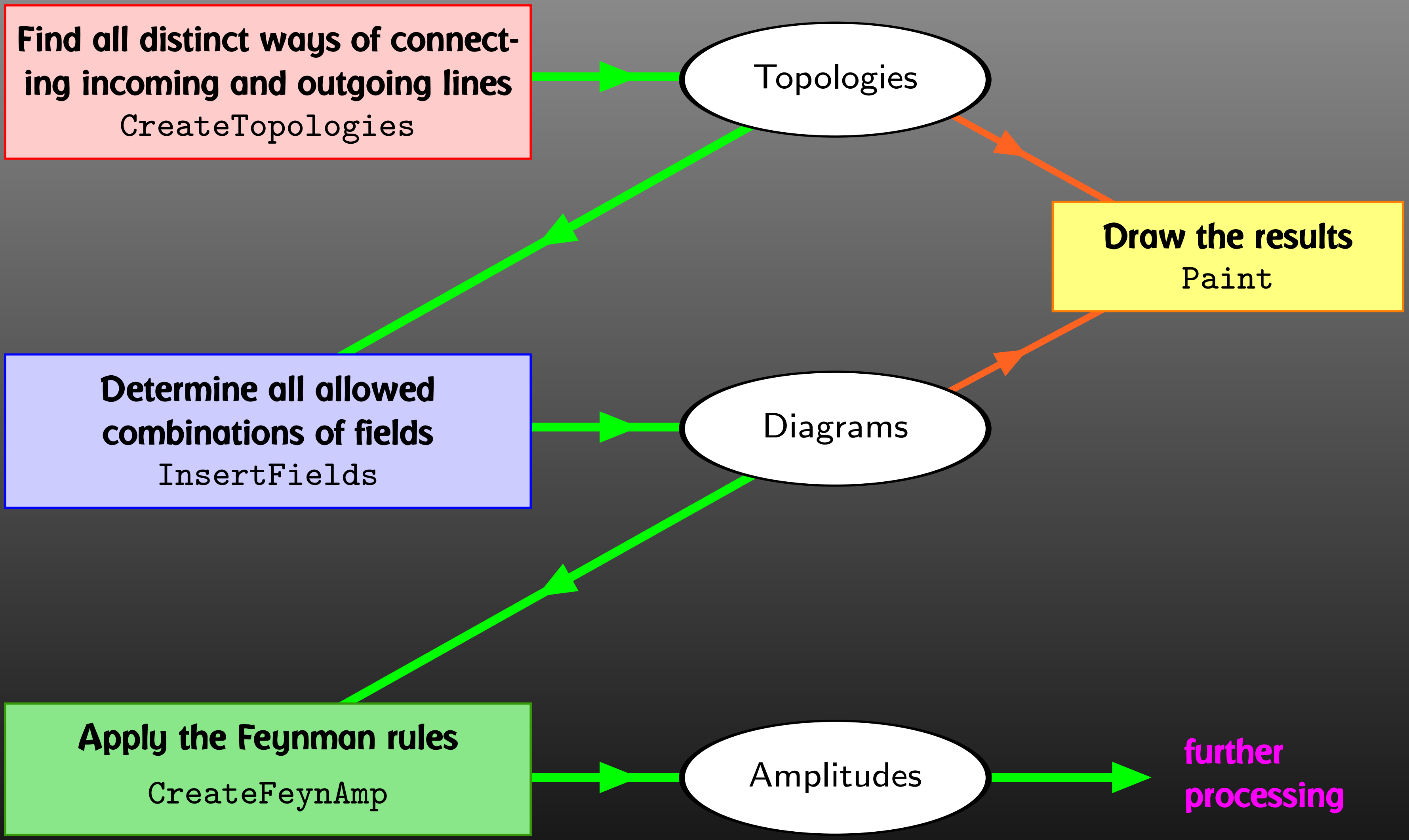
Numerical Evaluation:

- Convert Mathematica output to Fortran code
- Supply a driver program
- Implementation of the integrals

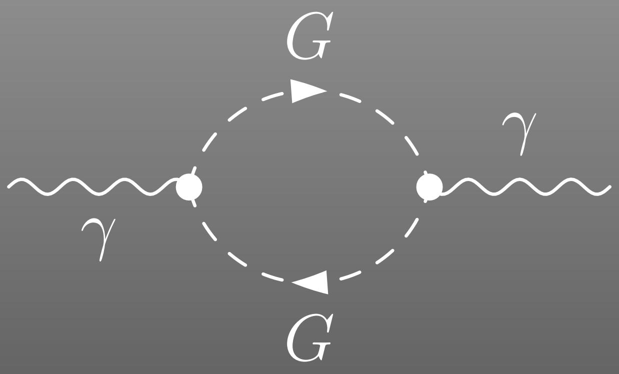
Symbolic manipulation (Computer Algebra) for the structural and algebraic operations.

Compiled high-level language (Fortran) for the numerical evaluation.

FeynArts


Find all distinct ways of connecting incoming and outgoing lines
CreateTopologies
Topologies
Draw the results
Paint
Determine all allowed combinations of fields
InsertFields
Diagrams
Apply the Feynman rules
CreateFeynAmp
Amplitudes
further processing

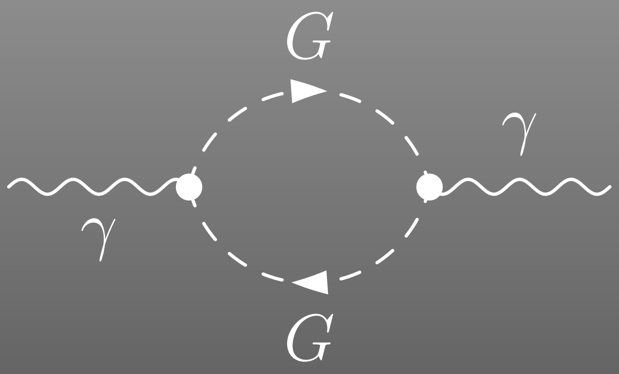
Sample CreateFeynAmp output



= `FeynAmp[` $\boxed{\textit{identifier}}$,
loop momenta,
generic amplitude,
insertions `]`

```
GraphID[Topology == 1, Generic == 1]
```

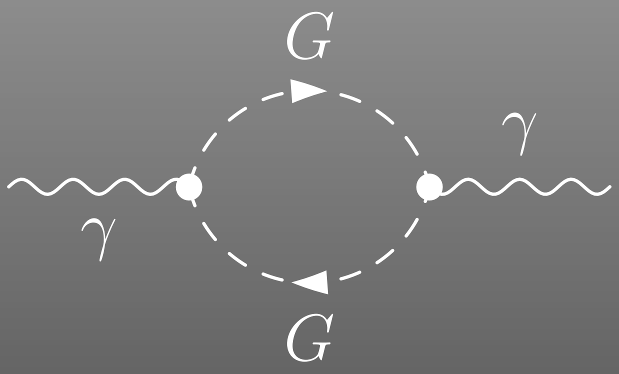
Sample CreateFeynAmp output



= `FeynAmp[` *identifier* ,
$\boxed{\textit{loop momenta}}$,
generic amplitude ,
insertions `]`

```
Integral[q1]
```

Sample CreateFeynAmp output



= FeynAmp[*identifier*,
loop momenta,
$\boxed{\textit{generic amplitude}}$,
insertions]

$\frac{\texttt{I}}{\texttt{32 Pi}^4}$ RelativeCF ....*prefactor*

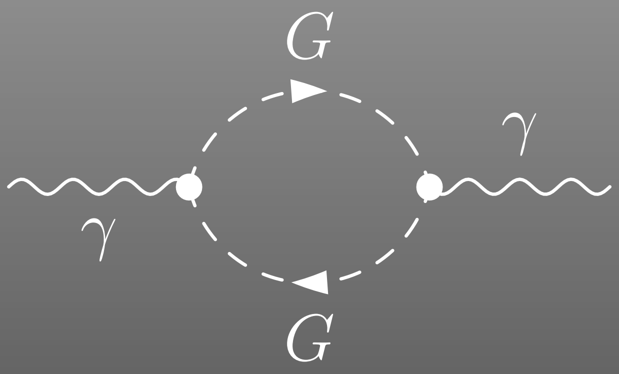
FeynAmpDenominator[$\frac{1}{\texttt{q1}^2 - \texttt{Mass[S[Gen3]]}^2}$,
$\frac{1}{(\texttt{-p1 + q1})^2 - \texttt{Mass[S[Gen4]]}^2}$] ....*loop denominators*

(p1 - 2 q1)[Lor1] (-p1 + 2 q1)[Lor2] ....*kin. coupling structure*

ep[V[1], p1, Lor1] ep*[V[1], k1, Lor2] ....*polarization vectors*

$\texttt{G}^{(0)}_{\texttt{SSV}}$[(Mom[1] - Mom[2])[KI1[3]]]
$\texttt{G}^{(0)}_{\texttt{SSV}}$[(Mom[1] - Mom[2])[KI1[3]]] ....*coupling constants*

Sample CreateFeynAmp output



$= \texttt{FeynAmp[}\ \textit{identifier}\,,$
$\textit{loop momenta}\,,$
$\textit{generic amplitude}\,,$
$\boxed{\textit{insertions}}\ \texttt{]}$

$\{\ \texttt{Mass[S[Gen3]]},$
$\quad \texttt{Mass[S[Gen4]]},$
$\quad G^{(0)}_{SSV}\texttt{[(Mom[1] - Mom[2])[KI1[3]]]},$
$\quad G^{(0)}_{SSV}\texttt{[(Mom[1] - Mom[2])[KI1[3]]]},$
$\quad \texttt{RelativeCF}\ \} \texttt{->}$
$\texttt{Insertions[Classes][\{MW, MW, I EL, -I EL, 2\}]}$

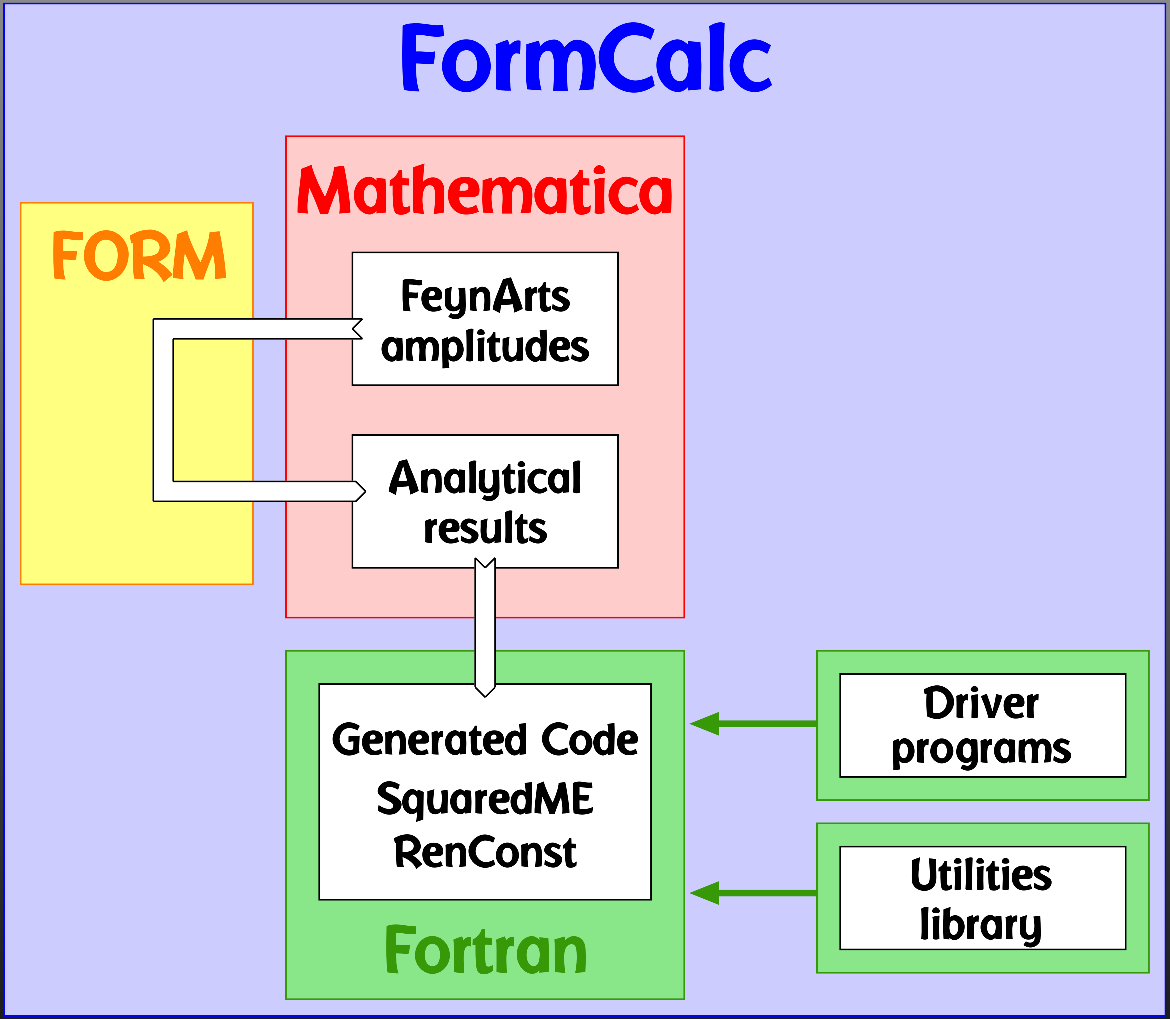
Algebraic Simplification

The amplitudes of `CreateFeynAmp` are in no good shape for direct numerical evaluation.

A number of steps have to be done analytically:

- contract indices as far as possible,
- evaluate fermion traces,
- perform the tensor reduction,
- add local terms arising from D·(divergent integral) (dim reg + dim red),
- simplify open fermion chains,
- simplify and compute the square of SU(N) structures,
- "compactify" the results as much as possible.

FormCalc Internals



FormCalc Output

A typical term in the output looks like

```
C0i[cc12, MW2, MW2, S, MW2, MZ2, MW2] *
  ( -4 Alfa2 MW2 CW2/SW2 S AbbSum16 +
    32 Alfa2 CW2/SW2 S^2 AbbSum28 +
    4 Alfa2 CW2/SW2 S^2 AbbSum30 -
    8 Alfa2 CW2/SW2 S^2 AbbSum7 +
    Alfa2 CW2/SW2 S (T-U) Abb1 +
    8 Alfa2 CW2/SW2 S (T-U) AbbSum29 )
```

🟩	= loop integral	🟥	= kinematical variables
🟪	= constants	🟨	= automatically introduced abbreviations

Abbreviations

Outright factorization is usually out of question.
Abbreviations are necessary to reduce size of expressions.

```
AbbSum29 = Abb2 + Abb22 + Abb23 + Abb3

        Abb22 = Pair1 Pair3 Pair6

              Pair3 = Pair[e[3],k[1]]
```

The full expression corresponding to `AbbSum29` is

```
Pair[e[1],e[2]] Pair[e[3],k[1]] Pair[e[4],k[1]] +
Pair[e[1],e[2]] Pair[e[3],k[2]] Pair[e[4],k[1]] +
Pair[e[1],e[2]] Pair[e[3],k[1]] Pair[e[4],k[2]] +
Pair[e[1],e[2]] Pair[e[3],k[2]] Pair[e[4],k[2]]
```

FormCalc 7

New Features:

- Analytic tensor reduction,
- Unitarity methods (OPP),
- Improved code generation,
- Command-line parameters for model initialization,
  MSSM (SM) initialization via FeynHiggs.
- Auxiliary functions for operator matching.

Cuba:

- Built-in Parallelization.

Analytic Tensor Reduction

Work done in collaboration with S. Agrawal.

Passarino-Veltman reduction is still useful. So far:

- introduction of tensor coefficients in FormCalc, e.g.

$$\int \mathrm{d}^4 q \, \frac{q_\mu q_\nu}{D_0 D_1} \sim B_{\mu\nu} = g_{\mu\nu} B_{00} + p_\mu p_\nu B_{11}$$

- complete reduction to scalars only numerically in LoopTools.

Available now: Analytic Reduction in FormCalc.

```
CalcFeynAmp[..., PaVeReduce -> True]
```

Analytic Tensor Reduction

Reduction formulas from Denner & Dittmaier, hep-ph/0509141. Not straightforward to implement in FORM.

Apart from analytic considerations, this is useful e.g. for low-energy observables, where small momentum transfer may lead to numerical instabilities in numerical reduction, as in:

$$B_\mu = p_\mu B_1 \quad \text{for} \quad p \to 0$$

Unless FormCalc finds a way to cancel it immediately, the inverse Gram determinant appears wrapped in `IGram` in the output, so is available for further modifications.

Unitarity Methods

Work done in collaboration with E. Mirabella.

We employ the OPP (Ossola, Papadopoulos, Pittau) methods as implemented in the two libraries CutTools and Samurai.

Instead of introducing tensor coefficients, the numerator is put into a subroutine which is sampled by the OPP function, as in:

$$\varepsilon_1^\mu \varepsilon_2^\nu B_{\mu\nu}(p, m_1^2, m_2^2) = B_{\text{cut}}(2, N, p, m_1^2, m_2^2)$$

where

$$N(q_\mu) = (\varepsilon_1 \cdot q)\,(\varepsilon_2 \cdot q)$$

Unitarity Methods

So far tested on a handful of $2 \to 2$ and $2 \to 3$ processes, get agreement to about 10 digits.

Interfacing with CutTools and Samurai quite similar, handled by preprocessor (no re-generation of code necessary).

Performance somewhat wanting as of now, Passarino-Veltman beats OPP hands down in the processes we looked at.

Main problem: OPP integrals are evaluted for every helicity configuration, but only once in Passarino-Veltman decomposition.

OPP optimization is work in progress.

Optimizing OPP Performance

- Option to specify the N in N-point up to which Passarino–Veltman is used, above OPP.
- Minimize OPP calls to reduce sampling effort, e.g. by collecting denominators, as in:

$$\frac{N_4}{D_0 D_1 D_2 D_3} + \frac{N_3}{D_0 D_1 D_2} \to \frac{N_4 + D_3 N_3}{D_0 D_1 D_2 D_3}$$

Move helicity sum into numerator in interference term:

$$\sum_\lambda 2\,\mathrm{Re}\,\mathcal{M}_0^* \underbrace{\int \mathrm{d}^4 q \frac{N}{D\dots}}_{\sim \mathcal{M}_1} = \int \mathrm{d}^4 q \frac{\sum_\lambda 2\,\mathrm{Re}\,\mathcal{M}_0^* N}{D\dots}$$

Optimizing OPP Performance

- Fermion chains evaluated in single function call:

$$\langle u|\,\sigma_\mu\overline{\sigma}_\nu\sigma_\rho\,|v\rangle\, k_1^\mu k_2^\nu k_3^\rho = \langle u|\, k_1\overline{k}_2 k_3\,|v\rangle$$

$$\textbf{old} = \texttt{SxS}(u,\ \texttt{VxS}(k_1,\ \texttt{BxS}(k_2,\ \texttt{VxS}(k_3,\ v))))$$

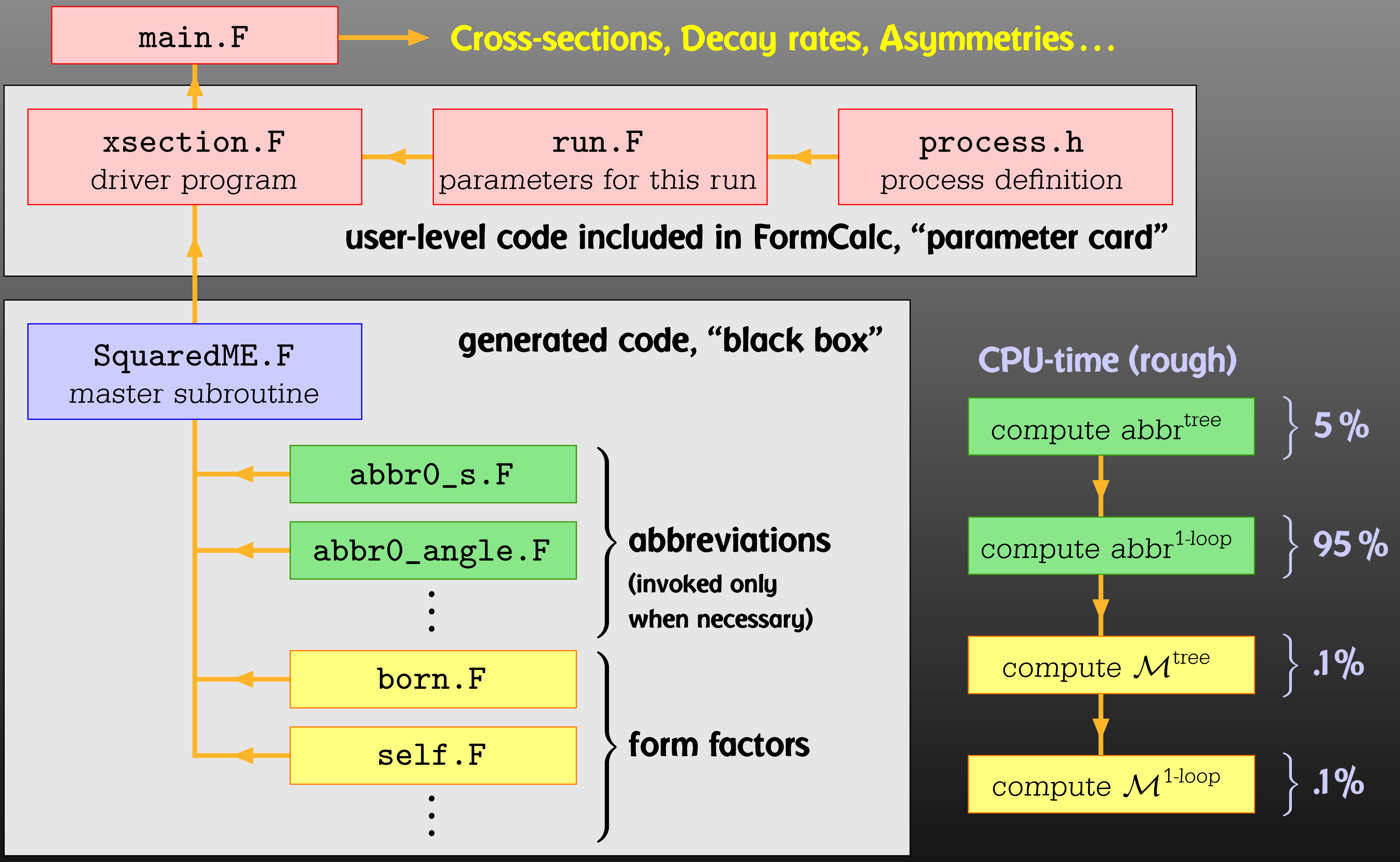
$$\textbf{new} = \texttt{Chain}(6, \underbrace{u + \texttt{JC}\,(k_1 + \texttt{JC}\,(k_2 + \texttt{JC}\,(k_3 + \texttt{JC}\,v)))}_{\text{single integer}}\,)$$

- Take into account helicity information for massless fermions, as in:

$$\texttt{Dcut}(3, N, 1 - \texttt{Hel1}, \ldots)$$

Evaluate integrals only if “hel-delta” argument is non-zero.

Numerical Evaluation in Fortran


main.F
Cross-sections, Decay rates, Asymmetries . . .
xsection.F
driver program
run.F
parameters for this run
process.h
process definition
user-level code included in FormCalc, “parameter card”
SquaredME.F
master subroutine
generated code, “black box”
abbr0_s.F
abbr0_angle.F
abbreviations
(invoked only
when necessary)
born.F
self.F
form factors
CPU-time (rough)
compute abbr$^{\text{tree}}$
5 %
compute abbr$^{\text{1-loop}}$
95 %
compute $\mathcal{M}^{\text{tree}}$
.1%
compute $\mathcal{M}^{\text{1-loop}}$
.1%

Code generation

Currently: Output in Fortran.
Code generator is rather sophisticated by now, e.g.

- Expressions too large for Fortran are split into parts, as in

```
var = part1
var = var + part2
...
```

- High level of optimization, e.g. common subexpressions are pulled out and computed in temporary variables.
- Many ancillary functions make code generation versatile and highly automatable, such that the resulting code needs few or no changes by hand.

Example: a significant part of FeynHiggs has been generated this way.

Improvements in Code Generation

- **Output in C** largely finished, makes integration into C/C++ codes easier and allows for GPU programming.
- **Loops and tests handled through macros,** e.g.

```
LOOP(var, 1,10,1)
ENDLOOP(var)
```

- Main subroutine `SquaredME` now **sectioned by comments,** to aid **automated substitution** e.g. with `sed`, e.g.

```
* BEGIN VARDECL
* END VARDECL
```

- Introduced **data types** `RealType` **and** `ComplexType` for better abstraction, can e.g. be changed to different precision.

Command-line parameters for model initialization

Extension of command-line argument parsing:

```
    run :arg1 :arg2 ... uuuuu 0,1000
```

The ':'-arguments are passed to model initialization code.

Internal routines in `xsection.F` accordingly have additional parameters `argv`, `argc`.

Application: FeynHiggs as Frontend for FormCalc-generated code (`model_fh.F`)

```
    run :fhparameterfile :fhflags uuuuu 0,1000
```

- FeynHiggs initializes MSSM (SM) parameters and passes them to FormCalc code.
- No duplication of initialization code.
- Parameters consistent between Higgs-mass and cross-section computation.

Aiding Operator Matching

As numerical calculations are done mostly using Weyl-spinor chains, there has been a paradigm shift for Dirac chains to make them better suited for analytical purposes, e.g. the extraction of Wilson coefficients.

- The `FermionOrder` option of `CalcFeynAmp` implements Fierz methods for Dirac chains, allowing the user to force fermion chains into any desired order. This includes the `Colour` method which brings the spinors into the same order as the external colour indices.
- The `Antisymmetrize` option allows the choice of completely antisymmetrized Dirac chains, i.e. $\texttt{DiracChain}[-1,\mu,\nu] = \sigma_{\mu\nu}$.
- The `Evanescent` option tracks operators before and after Fierzing for better control of ε-dimensional terms.

Cuba Parallelization: Design Considerations

- **1 Master, N workers on N-core system.**
  Master generates all samples, thus no issues with seeding random-number generators.
- **No parallelization across the network (e.g. via MPI).**
  OS functions only, no extra software needed.
  Mathematica separate: re-define `MapSample` e.g. by `ParallelMap`.
- **Uses internal cores ‘only’, thus e.g. 4 or 8.**
  (Many) more cores not necessarily useful since speed-ups not expected to be linear.
- **Auto-detect # of cores + load at run-time.**
  User control through environment variable `CUBACORES` (Condor).
  No re-compile necessary.

fork vs. pthread_create

- `pthread_create` creates additional thread in same memory space.
- `fork` creates completely independent process.
- Must use `fork` for non-reentrant integrands.
  Reentrancy cannot be fully controlled e.g. in Fortran.
- Keep `fork` calls minimal: 'Spinning Threads' method = fork N times at entry into Cuba routine.

  No `fork` in Windows, Cygwin emulates but quite slow.
  Despite 'copy-on-write' (Linux), `fork` is moderately 'expensive' even on Linux/MacOS.
- Master-worker communication:
  (if available:) shared memory for samples,
  socketpair I/O for control information (creates scheduling hint for kernel, too).

Implementation

- Main sampling routine `DoSample` already abstracted in Cuba 1, 2 since C/C++ and Mathematica implementations very different.
- `DoSample` straightforward to parallelize on N cores:

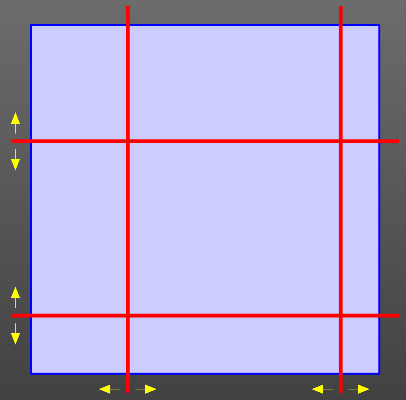
Serial	$\to$ sample n points
Parallel	$\to$ send $\lceil n/N \rceil$ points to core 1
	$\to$ send $\lceil n/N \rceil$ points to core 2
	$\to \ldots$

- Fill fewer cores if not enough samples.
- Divonne: Parallelizing `DoSample` alone not satisfactory. Speed-ups generally $\lesssim$ 1.5.
  Partitioning phase significant. Originally recursive, had to 'un-recurse' algorithm first.

Divonne Algorithm

- **PHASE 1 – Partitioning**
  - For each subregion, 'actively' determine $\sup f$ and $\inf f$ using methods from numerical optimization.
  - Move 'dividers' around until all subregions have approximately equal spread, defined as

$$\text{Spread}(r) = \frac{1}{2}\,\text{Vol}(r)\left(\sup_{\vec{x}\in r} f(\vec{x}\,) - \inf_{\vec{x}\in r} f(\vec{x}\,)\right).$$



- **PHASE 2 – Sampling**
  Sample the subregions independently with the same number of points each. The latter is extrapolated from the results of Phase 1.
- **PHASE 3 – Refinement**
  Further subdivide or sample again if results from Phase 1 and 2 do not agree within their error.

Inefficiencies

Assess parallelization efficiency through

$$\text{speed-up} = \frac{t_{\text{serial}}}{t_{N\text{-cores}}} \qquad \text{ideally} = N.$$

- Parallelization overhead = Extra time for communication, scheduling efficiency etc.
  Overhead can be estimated through $t_{\text{serial}}/t_{1\text{-core}} < 1$.
- Load levelling = Keeping cores busy. If only $N - n$ busy, absolute timing may be ok but N-core speed-up lousy.
- Caveat: Hyperthreading, e.g. i7 has 8 virtual, 4 real cores.

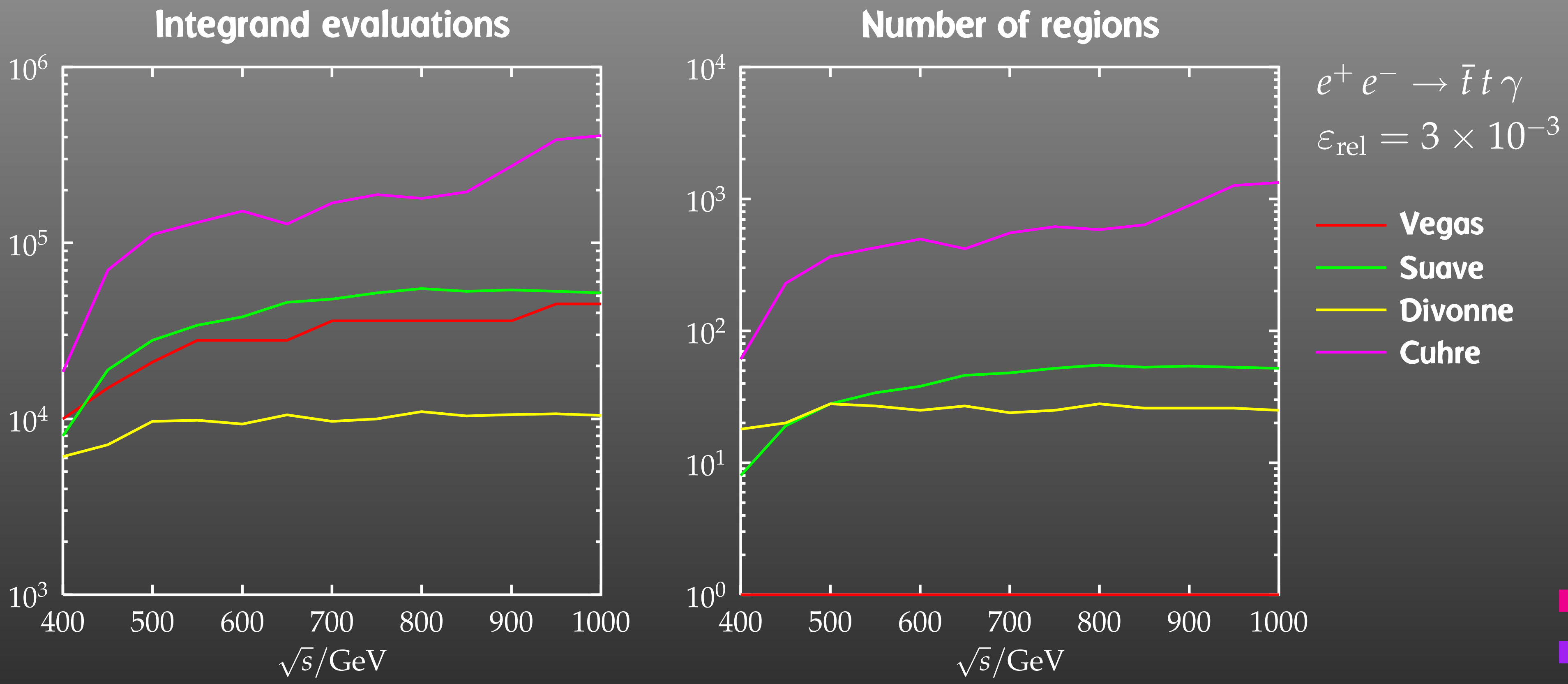
Speed-ups will obviously depend on the 'cost' of the integrand: The more time a single integrand evaluation takes, the better speed-ups can be expected to achieve.

Timing Measurements

Timing measurements delicate on multicore systems:

- System timer (even `ualarm`) has granularity.
- Cannot use timer interrupt directly in integrand delay, accumulates too large errors.
- First calibrate delay loop over sufficiently long time interval.
- Use same calibrated value per machine for all runs.
- Repeat integrations such that each measurement takes a reasonable minimum amount of time (to minimize measurement errors).
- Disable processes like `condor_start`, `autonice`, etc.

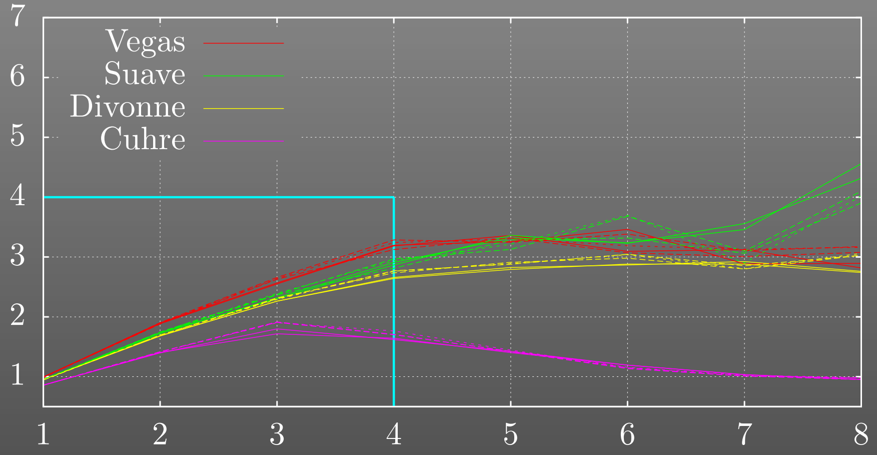
Cuba Comparison



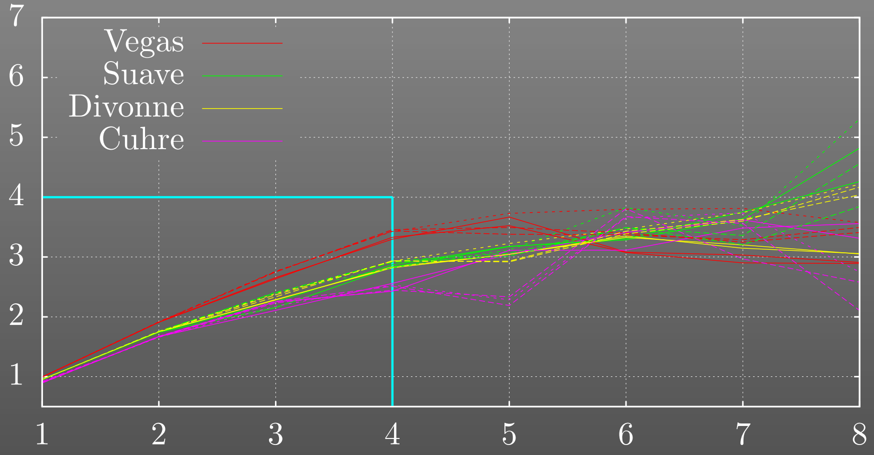
‘Gauge’ integration problem first:

- Compute with all four routines.
- Check whether results are consistent.
- Select fastest algorithm.

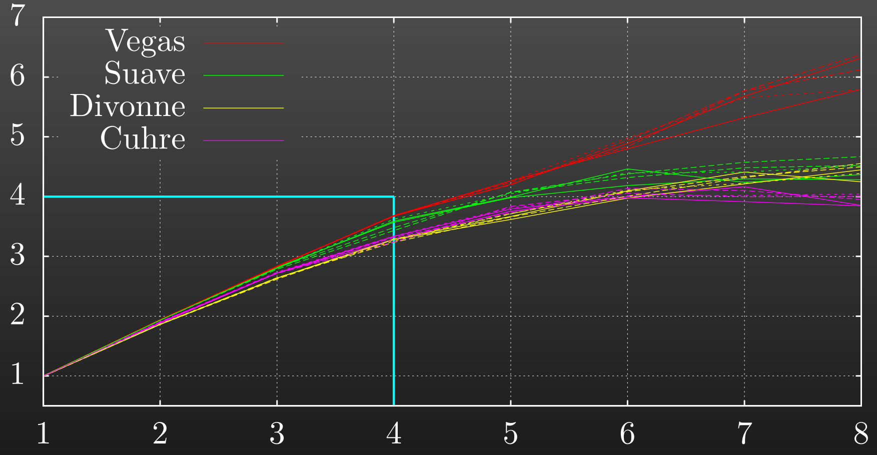
Timing Results



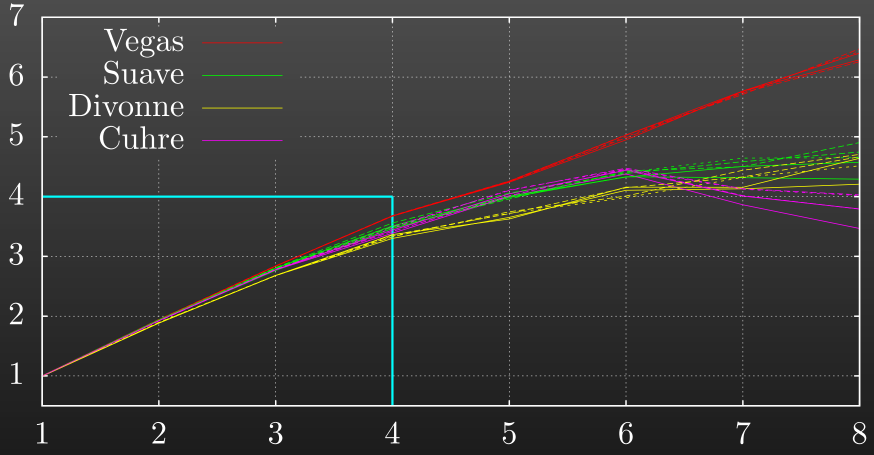
integrand 1, delay 10 μsec



integrand 11, delay 10 μsec



integrand 1, delay 1000 μsec



integrand 11, delay 1000 μsec

$$f_1 = \sin x\ \cos y\ \exp z$$

$$\varepsilon_{\text{rel}} = 10^{-4}$$

$$f_{11} = \Theta(1 - x^2 - y^2 - z^2)$$

Summary

New Features in FormCalc 7: feynarts.de/formcalc

- Analytic tensor reduction in `CalcFeynAmp`,
- Unitarity (OPP) methods using either the Samurai or CutTools library,
- Improved code generation,
- Command-line parameters for model initialization,
- Initialization of MSSM parameters via FeynHiggs,
- Options aiding operator matching (Fierz, antisymmetry, evanescent operators).

Cuba: feynarts.de/cuba

- Built-in Parallelization available simply by compiling with Cuba 3.