# Nested Sums and Multi-Scale Multi-Loop Integrals

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in collaboration with
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**I. Physics:**
$e^+e^- \to 3$ **jets at NNLO**

**II. Mathematics:**
**Nested sums and Hopf algebras**

**III. Computer science:**
**Symbolic calculation in C++**

# Perturbative NNLO calculations

The experimental precision has to be matched with an improvement in the accuracy of theoretical predictions.

Fully differential NNLO programs for

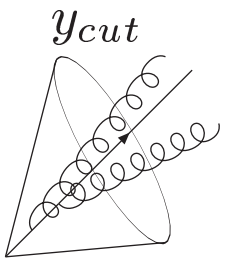
- Bhabha scattering
- $pp \to 2$ jets
- $e^+e^- \to 3$ jets

which allow the calculation of any infrared safe observable.

# $e^+e^- \to 3$ jets

- Measurement of $\alpha_s$ using data of $e^+e^- \to 3$ jets. A NNLO calculation is expected to reduce the theoretical error in the extraction of $\alpha_s$ down to 1%.

- A NNLO calculation models the jet structure more accurately and should allow to improve the knowledge on the interplay between perturbative QCD and power corrections.



# Recent progress in NNLO calculations

- Two loop master integrals: Double boxes, crossed double boxes, pentaboxes
  - Mellin-Barnes: V.A. Smirnov, J.B. Tausk
  - Differential equations: T. Gehrmann and E. Remiddi
  - Negative dimensions: C. Anastasiou, N. Glover and C. Oleari
- Two loop amplitudes:
  - Bhabha: Z. Bern, L. Dixon and A. Ghinculov
  - $pp \to 2$ jets: C. Anastasiou, N. Glover, C. Oleari and M. Tejeda-Yeomans
- Singular limits:
  - Double unresolved: J. Campbell and N. Glover, S. Catani and M. Grazzini
  - One-loop + unresolved: Z. Bern, V. Del Duca, W. Kilgore and C. Schmidt, D. Kosower and P. Uwer
  - Pole structure of two-loop: S. Catani
- Numerical cross-checks:
  - Sector decomposition: Th. Binoth and G. Heinrich
  - Difference equations: S. Laporta

# To-Do list

- Calculation of the two-loop amplitudes for $e^+e^- \to 3$ jets.

  Requires: Tensor reduction. The result will depend on two ratios of scales, for example $s_{12}/s_{123}$ and $s_{23}/s_{123}$.
  The calculated two-loop amplitudes for Bhabha scattering and $pp \to 2$ jets depend only on one ratio $x = s/t$.

- Cancellation of IR divergences has to be done before any Monte Carlo integration.

  Requires: Extension of the subtraction or slicing method to NNLO. Analytic integration over unresolved regions or dipole phase space.

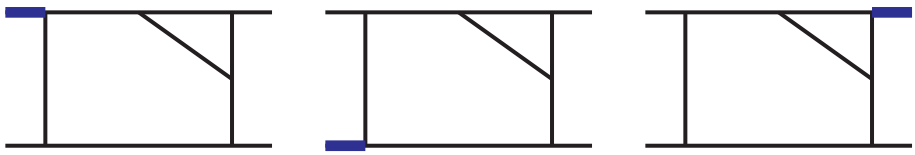
- The final numerical computer program.

  Requires: Stable and efficient numerical methods.

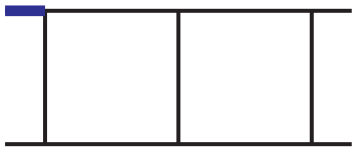
# Two-loop diagrams and how we break them into little pieces

## Basic topologies at two loops

- penta-box



- double-box



- nonplanar-box

# Tensor reduction

The standard approach:

- Using Schwinger parameters a tensor integral can be related to a scalar integral with higher powers of the propagators and different values of $D$

  (Tarasov '96).

- Integration-by-parts, Lorentz-invariance identities and form-factor relations can be used to reduce the powers of the propagators and to relate master integrals in higher dimensions to master integrals in $D = 4 - 2\varepsilon$ dimensions.

  't Hooft, Veltman '72; Chetyrkin, Tkachov '81;

  Gehrmann, Remiddi '99;

  Larin '81; Moch, Vermaseren '99.

- Complicated diagrams mapped onto simpler ones.

- This has to be done for each topology.

# Tensor reduction

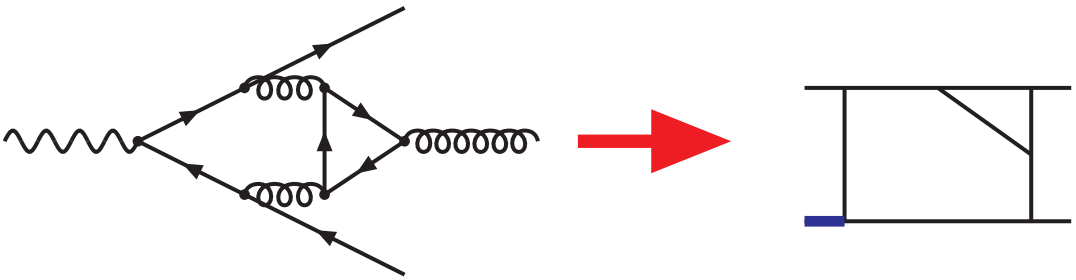
Solve directly the scalar integrals with arbitrary powers of the propagators and arbitrary dimension:

- Transformation of the integral into a mathematical object. Depends on the topology of the original integral, but is rather easy to perform.

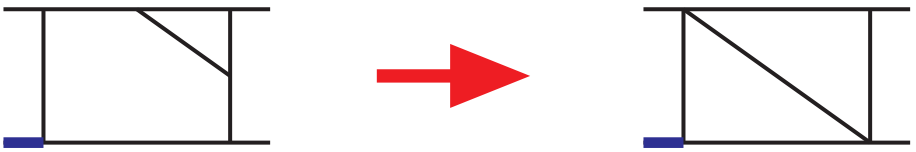
- Expansion of this mathematical object in $\varepsilon$, using generic algorithms. The algorithms are derived from the mathematical properties of the class of objects and independent of the original topology.

# Simple example

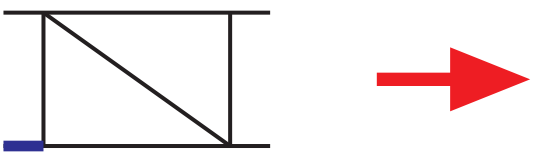
- Transform a diagram into a basic topology



- Reduction of the penta-box to the C-topology



- Evaluation of the C-topology



multiple polylogs

# The two-loop C-topology

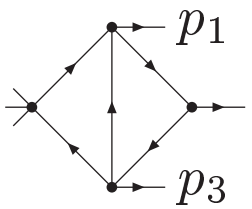
The integral reads :

$$\int \frac{d^D k_1}{i\pi^{D/2}} \int \frac{d^D l_5}{i\pi^{D/2}} \frac{1}{(-k_1^2)^{\nu_1}} \frac{1}{(-l_2^2)^{\nu_2}} \frac{1}{(-l_3^2)^{\nu_3}} \frac{1}{(-k_4^2)^{\nu_4}} \frac{1}{(-l_5^2)^{\nu_5}}$$

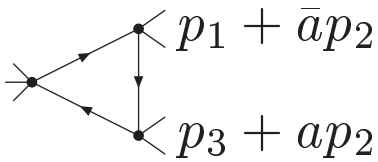
with

$$\begin{aligned} l_2 &= k_1 + l_5 - p_1, \\ l_3 &= l_2 - p_2, \\ k_4 &= k_1 - p_{123}. \end{aligned}$$

Reduction to a one-loop triangle :




$$= c \int_0^1 da\, a^{\nu_2 - 1} \bar{a}^{\nu_3 - 1}$$



# The two-loop C-topology

The result for the C-topology in arbitrary dimensions and with arbitrary powers of the propagators:

$$
\frac{\Gamma(2m-2\varepsilon-\nu_{1235})\Gamma(1+\nu_{1235}-2m+2\varepsilon)\Gamma(2m-2\varepsilon-\nu_{2345})\Gamma(1+\nu_{2345}-2m+2\varepsilon)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(\nu_3)\Gamma(\nu_4)\Gamma(\nu_5)\Gamma(3m-3\varepsilon-\nu_{12345})}
$$

$$
\cdot\frac{\Gamma(m-\varepsilon-\nu_5)\Gamma(m-\varepsilon-\nu_{23})}{\Gamma(2m-2\varepsilon-\nu_{235})}\,(-s_{123})^{2m-2\varepsilon-\nu_{12345}}\sum_{i_1=0}^{\infty}\sum_{i_2=0}^{\infty}\frac{x_1^{i_1}}{i_1!}\frac{x_2^{i_2}}{i_2!}
$$

$$
\cdot\left[\frac{\Gamma(i_1+\nu_3)\Gamma(i_2+\nu_2)\Gamma(i_1+i_2-2m+2\varepsilon+\nu_{12345})\Gamma(i_1+i_2-m+\varepsilon+\nu_{235})}{\Gamma(i_1+1-2m+2\varepsilon+\nu_{1235})\Gamma(i_2+1-2m+2\varepsilon+\nu_{2345})\Gamma(i_1+i_2+\nu_{23})}\right.
$$

$$
-x_1^{2m-2\varepsilon-\nu_{1235}}
$$

$$
\cdot\frac{\Gamma(i_1+2m-2\varepsilon-\nu_{125})\Gamma(i_2+\nu_2)\Gamma(i_1+i_2+\nu_4)\Gamma(i_1+i_2+m-\varepsilon-\nu_1)}{\Gamma(i_1+1+2m-2\varepsilon-\nu_{1235})\Gamma(i_2+1-2m+2\varepsilon+\nu_{2345})\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{15})}
$$

$$
-x_2^{2m-2\varepsilon-\nu_{2345}}
$$

$$
\cdot\frac{\Gamma(i_1+\nu_3)\Gamma(i_2+2m-2\varepsilon-\nu_{345})\Gamma(i_1+i_2+\nu_1)\Gamma(i_1+i_2+m-\varepsilon-\nu_4)}{\Gamma(i_1+1-2m+2\varepsilon+\nu_{1235})\Gamma(i_2+1+2m-2\varepsilon-\nu_{2345})\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{45})}
$$

$$
+x_1^{2m-2\varepsilon-\nu_{1235}}x_2^{2m-2\varepsilon-\nu_{2345}}
$$

$$
\cdot\frac{\Gamma(i_1+2m-2\varepsilon-\nu_{125})\Gamma(i_2+2m-2\varepsilon-\nu_{345})}{\Gamma(i_1+1+2m-2\varepsilon-\nu_{1235})\Gamma(i_2+1+2m-2\varepsilon-\nu_{2345})}
$$

$$
\left.\cdot\frac{\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{235})\Gamma(i_1+i_2+3m-3\varepsilon-\nu_{12345})}{\Gamma(i_1+i_2+4m-4\varepsilon-\nu_{12345}-\nu_5)}\right],
$$

with $D = 2m - 2\varepsilon$, $x_1 = (-s_{12})/(-s_{123})$ and $x_2 = (-s_{23})/(-s_{123})$.

This sum can be expanded systematically in $\varepsilon$.

# Higher transcedental functions

We need the expansion of higher transcedental functions, where the expansion parameter $\varepsilon$ occurs in the Pochhammer symbols.

Hypergeometric function:

$$ {}_2F_1(a,b;c,x_0) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{x_0^n}{n!} $$

First Appell function:

$$ F_1(a,b_1,b_2;c;x_1,x_2) $$
$$ = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(a)_{m_1+m_2} (b_1)_{m_1} (b_2)_{m_2}}{(c)_{m_1+m_2}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!} $$

Second Appell function:

$$ F_2(a,b_1,b_2;c_1,c_2;x_1,x_2) $$
$$ = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(a)_{m_1+m_2} (b_1)_{m_1} (b_2)_{m_2}}{(c_1)_{m_1} (c_2)_{m_2}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!} $$

Here $(a)_n = \Gamma(a+n)/\Gamma(a)$ denotes the Pochhammer symbol.

But : These higher transcedental functions are not complete.

# Introducing nested sums

- Definition of nested sums

$$Z(n; m_1, ..., m_k; x_1, ..., x_k) =$$
$$= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} Z(i-1; m_2, ..., m_k; x_2, ..., x_k),$$
$$Z(n) = 1 \quad \text{for } n \geq 0.$$

- Multiple polylogarithms are a special subset
- Euler-Zagier sums are a special subset
- The nested sums form a Hopf algebra

These methods have already been applied to the integration of subtraction terms occuring in the dipole formalism with massive fermions
(L.Phaf and S.W.).

Z-sums interpolate between multiple polylogarithms and Euler-Zagier sums.

# Definition of the nested sums

Z- and S-sums are defined as:

$$Z(n; m_1, ..., m_k; x_1, ..., x_k) =$$

$$= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} Z(i-1; m_2, ..., m_k; x_2, ..., x_k),$$

$$Z(n) = 1 \quad \text{for } n \geq 0,$$

$$S(n; m_1, ..., m_k; x_1, ..., x_k) =$$

$$= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} S(i; m_2, ..., m_k; x_2, ..., x_k),$$

$$S(n) = 1 \quad \text{for } n > 0,$$

$k$ is called the depth, $w = m_1 + ... + m_k$ the weight.

Example:

$$Z(n; m_1, m_2, m_3; x_1, x_2, x_3) =$$

$$= \sum_{i_1=1}^{n} \sum_{i_2=1}^{i_1-1} \sum_{i_3=1}^{i_2-1} \frac{x_1^{i_1}}{{i_1}^{m_1}} \frac{x_2^{i_2}}{{i_2}^{m_2}} \frac{x_3^{i_3}}{{i_3}^{m_3}} \quad =$$

# Special cases

For $n = \infty$ the Z-sums are the multiple polylogarithms of Goncharov:

$$Z(\infty; m_1, ..., m_k; x_1, ..., x_k) \quad = \quad \mathrm{Li}_{m_k,...,m_1}(x_k, ..., x_1)$$

For $x_1 = ... = x_k = 1$ the definition reduces to the Euler-Zagier sums:

$$Z(n; m_1, ..., m_k; 1, ..., 1) \quad = \quad Z_{m_1,...,m_k}(n)$$

For $n = \infty$ and $x_1 = ... = x_k = 1$ the sum is a multiple $\zeta$-value:

$$Z(\infty; m_1, ..., m_k; 1, ..., 1) \quad = \quad \zeta(m_k, ..., m_1)$$

The S-sums reduce for $x_1 = ... = x_k = 1$ to harmonic sums:

$$S(n; m_1, ..., m_k; 1, ..., 1) \quad = \quad S_{m_1,...,m_k}(n)$$

# Goncharov's multiple polylogarithms

The multiple polylogarithms have extensively been studied by Borwein, Bradley, Broadhurst and Lisonek. The multiple polylogarihms contain as subsets the classical polylogarithms

$$\mathrm{Li}_n(x),$$

Nielsen's generalized polylogarithms

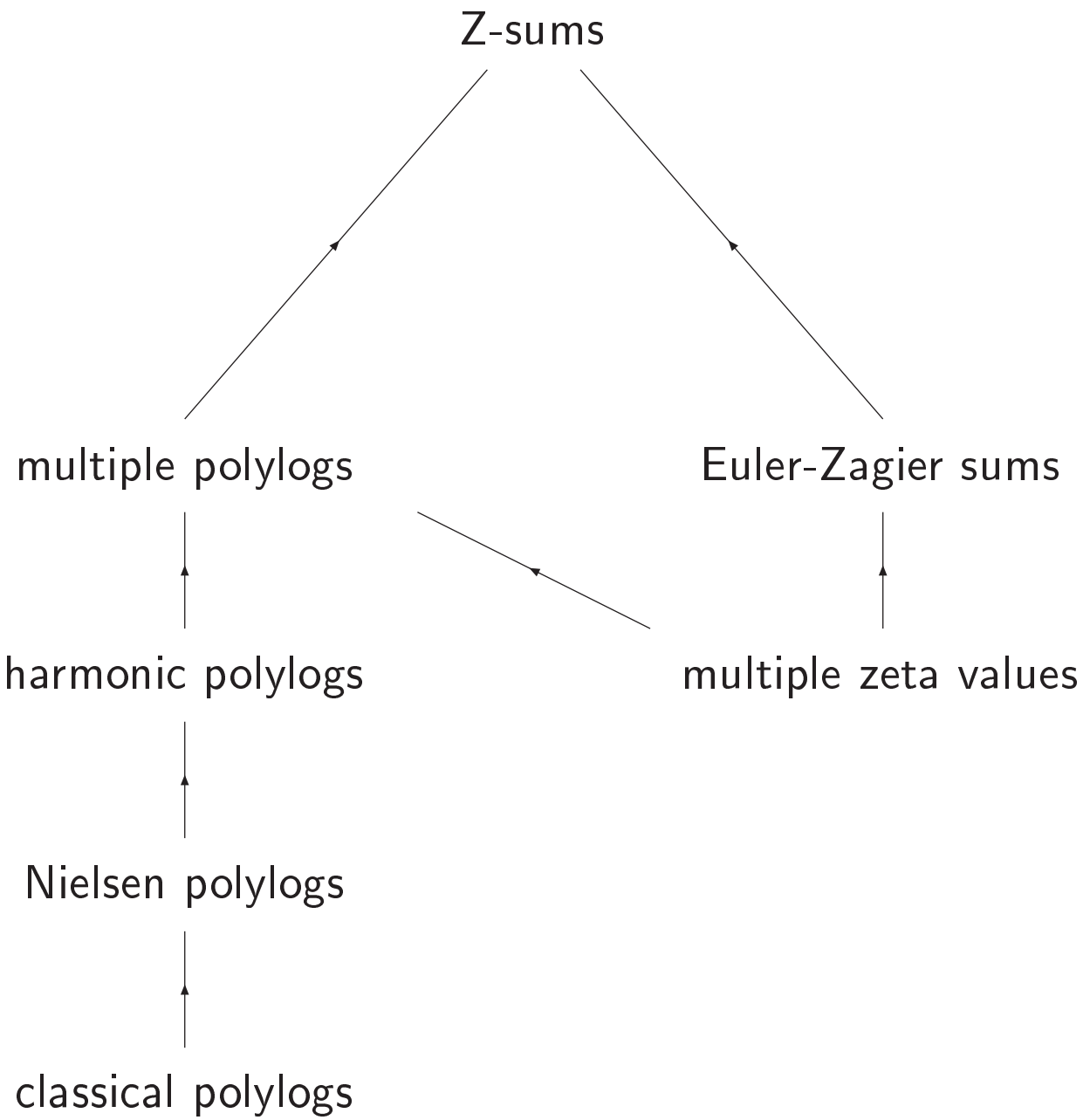
$$S_{n,p}(x) \quad = \quad \mathrm{Li}_{1,...,1,n+1}(\underbrace{1,...,1}_{p-1},x),$$

the harmonic polylogarithms of Remiddi and Vermaseren

$$H_{m_1,...,m_k}(x) \quad = \quad \mathrm{Li}_{m_k,...,m_1}(\underbrace{1,...,1}_{k-1},x)$$

and the two-dimensional harmonic polylogarithms introduced recently by Gehrmann and Remiddi.

# Inheritance



# Expansion of Gamma functions

Euler-Zagier sums (or harmonic sums) occur in the expansion for $\Gamma$ functions: For positive integers $n$ we have

$$\Gamma(n+\varepsilon) = \Gamma(1+\varepsilon)\Gamma(n)$$
$$\cdot \left(1 + \varepsilon Z_1(n-1) + \varepsilon^2 Z_{11}(n-1) + \varepsilon^3 Z_{111}(n-1)\right.$$
$$\left. + \ldots + \varepsilon^{n-1} Z_{11\ldots1}(n-1)\right).$$

Z-sums interpolate between Goncharov's multiple polylogarithms and Euler-Zagier sums.

# Multiplication

A product of two nested sums with the same upper summation index can be converted into single sums:

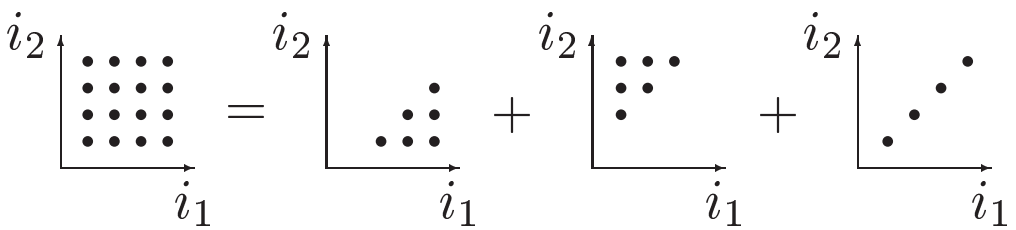
$$Z(n;m_1,...,m_k;x_1,...,x_k)Z(n;m'_1,...,m'_l;x'_1,...,x'_l) =$$

$$\sum_{i_1=1}^{n} \frac{x_1^{i_1}}{i_1^{m_1}} Z(i_1-1;m_2,...;x_2,...)Z(i_1-1;m'_1,...;x'_1,...)$$

$$+\sum_{i_2=1}^{n} \frac{x'^{\,i_2}_1}{i_2^{m'_1}} Z(i_2-1;m_1,...;x_1,...)Z(i_2-1;m'_2,...;x'_2,...)$$

$$+\sum_{i=1}^{n} \frac{(x_1x'_1)^i}{i^{m_1+m'_1}} Z(i-1;m_2,...;x_2,...)Z(i-1;m'_2,...;x'_2,...)$$

Sketch of the proof:

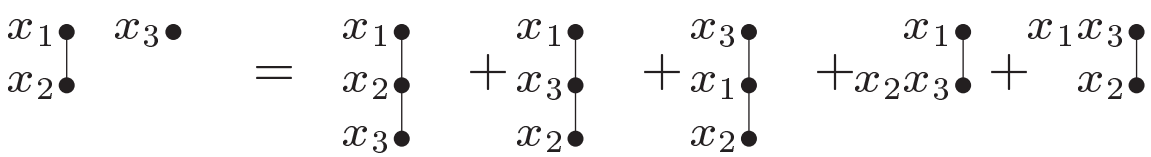



The sum over the square is replaced by the sum over the three regions on the r.h.s.

This defines an algebra structure for Z-sums !

# Example

$$
\begin{aligned}
Z(n; m_1, m_2; x_1, x_2) \cdot Z(n; m_3; x_3) = \\
= \quad & Z(n; m_1, m_2, m_3; x_1, x_2, x_3) \\
& + Z(n; m_1, m_3, m_2; x_1, x_3, x_2) \\
& + Z(n; m_3, m_1, m_2; x_3, x_1, x_2) \\
& + Z(n; m_1, m_2 + m_3; x_1, x_2 x_3) \\
& + Z(n; m_1 + m_3, m_2; x_1 x_3, x_2)
\end{aligned}
$$



# Hopf algebras

The Z-sums form actually a Hopf algebra.

- An algebra has a multiplication $\cdot$ and a unit $e$.
- A coalgebra has a comultiplication $\Delta$ and a counit $\bar{e}$.
- A Hopf algebra is an algebra and a coalgebra at the same time, such that the two structures are compatible with each other.

  In addition, there is an antipode $S$.

# Hopf algebras and renormalization of quantum field theories

Short-distance singularities of the perturbative expansion of quantum field theories require renormalization (Bogoliubov, Parasuik, Hepp, Zimmermann).

The combinatorics involved in the renormalization is governed by a Hopf algebra (Kreimer, Connes).

The model for this Hopf algebra is the Hopf algebra of rooted trees.

Also the Z-sums are described by the Hopf algebra of rooted trees.

# Algorithms

Conversion between Z-sums and S-sums

Multiplication:

$$Z(n; m_1, ...; x_1, ...) \cdot Z(n; m'_1, ...; x'_1, ...)$$

Sums involving $i$ and $n - i$:

$$\sum_{i=1}^{n-1} \frac{x_1^i}{i^{m_1}} Z(i-1; m_2 ...; x_2, ...) \frac{{x'_1}^{n-i}}{(n-i)^{m'_1}} Z(n-i-1; m'_2, ...; x'_2, ...)$$

Conjugations:

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x_0^i}{i^{m_0}} S(i; m_1, ..., m_k; x_1, ..., x_k)$$

Sums involving binomials and $n - i$:

$$-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x_1^i}{i^{m_1}} S(i; m_2 ...; x_2, ...) \frac{{x'_1}^{n-i}}{(n-i)^{m'_1}} S(n-i; m'_2, ...; x'_2, ...)$$

# Hypergeometric Functions

Expansion of hypergeometric functions:

$$ {}_2F_1(a+\varepsilon, b+\varepsilon; c+\varepsilon, x_0) = \sum_{n=0}^{\infty} \frac{(a+\varepsilon)_n (b+\varepsilon)_n}{(c+\varepsilon)_n} \frac{x_0^n}{n!} $$

- Synchronize the Pochhammer symbols using $\Gamma(x+1) = x\Gamma(x)$.
- Expand the $\Gamma$-functions in $\varepsilon$. This will introduce Euler-Zagier sums.
- Combine products of Euler-Zagier sums into single sums.
- Read out the harmonic polylogarithms.

# Implementation on a computer

Requirements on a computer algebra system:

- Efficiency in performance: Compilation
- Object-oriented, strong type checking
- Short development cycles: Interactive use and high-quality output
- Source code freely available

The GiNaC library allows symbolic calculation in C++ (Ch.Bauer, A.Frink and R.Kreckel).

gTybalt for interactive use and debugging (R. Marani and S.W.) .

# gTybalt

gTybalt is build on top of several other packages:

- GiNaC by Christian Bauer, Alexander Frink und Richard Kreckel as a C++ library for symbolic mathematical calculations.
- The numeric part of GiNaC is build on the CLN library by Bruno Haible.
- Cint by Masaharu Goto as a C++/C interpreter,
- Root by Rene Brun and Fons Rademakers for plots and graphics and
- TeXmacs by Joris van der Hoeven as editor for TeX-type output.

available at:
`http://www.fis.unipr.it/~stefanw/gtybalt.html`

# Benchmarks

Multiplication of two harmonic sums

$$S_{\underbrace{11\ldots1}_{k}}(n) \cdot S_{\underbrace{11\ldots1}_{k}}(n),$$

where each factor has $k$ "one"'s in the index field.

| $k$ | C++ | Form | Maple |
|---|---|---|---|
| 1 | $< 1$ | $< 1$ | $< 1$ |
| 2 | $< 1$ | $< 1$ | $< 1$ |
| 3 | $< 1$ | $< 1$ | $< 1$ |
| 4 | $< 1$ | $< 1$ | $< 1$ |
| 5 | $< 1$ | $< 1$ | $< 1$ |
| 6 | 1 | 2 | 4 |
| 7 | 7 | 11 | 29 |
| 8 | 40 | 58 | crashed |
| 9 | 230 | 323 | crashed |
| 10 | 1343 | 1816 | crashed |

Table 1: CPU time in seconds for the multiplication of two harmonic sums on a 300 MHz Pentium II.

# Conclusions and Outlook

- Solving loop integrals:
  - Transformation into a mathematical object.
  - Expansion of this object in $\varepsilon$.
- Spin-off: Expansion of higher transcedental functions.
- Technique: Hopf algebra of nested sums.
- Implementation: C++ using the GiNaC library.
- Spin-off: gTybalt
- Application to $e^+e^- \to 3$ jets