



Loops and Legs in QFT 2012, Wernigerode

# Modern Summation Technologies and the Calculation of 3-Loop Diagrams

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joint work with J. Blümlein, A. Hasselhuhn, F. Wissbrock (DESY),  
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# Example: 3-loop topologies of gluonic massive operator matrix elements with two fermion lines (unpolarized case)

$$D_\varepsilon(n) = \text{[diagram 1]} + \text{[diagram 2]} + \sim 80 \text{ further diagrams}$$

[by axodraw (J. Vermaseren)]

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↓ J. Blümlein, A. Hasselhuhn

$$D_\varepsilon(n) = \sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \pi 2^{\varepsilon+3} e^{-\frac{3\gamma\varepsilon}{2}} \Gamma(2-\varepsilon) \Gamma\left(\frac{\varepsilon}{2}+2\right) \Gamma\left(-\frac{3\varepsilon}{2}\right) \quad (\sim 2\text{GB})$$

$$\times \frac{(-1)^{j_1} (j_2+1) \Gamma\left(-\frac{\varepsilon}{2}+j_1+4\right) \Gamma(-j_1+n-2) \Gamma(\varepsilon-j_1-j_2+n-5)}{(\varepsilon-10)(\varepsilon-8)(\varepsilon-2)\varepsilon \Gamma\left(\frac{5}{2}-\varepsilon\right) \Gamma\left(\frac{\varepsilon+5}{2}\right) \Gamma\left(\frac{\varepsilon}{2}+n+1\right) \Gamma(-j_1-j_2+n-4)}$$

+  $\sim \mathbf{2400}$  further multi-sums

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$$D_\varepsilon(n) = \sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \pi^2 \varepsilon^{+3} e^{-\frac{3\gamma\varepsilon}{2}} \Gamma(2-\varepsilon) \Gamma\left(\frac{\varepsilon}{2}+2\right) \Gamma\left(-\frac{3\varepsilon}{2}\right) \quad (\sim 2\text{GB})$$

$$\times \frac{(-1)^{j_1} (j_2+1) \Gamma(-\frac{\varepsilon}{2}+j_1+4) \Gamma(-j_1+n-2) \Gamma(\varepsilon-j_1-j_2+n-5)}{(\varepsilon-10)(\varepsilon-8)(\varepsilon-2)\varepsilon \Gamma(\frac{5}{2}-\varepsilon) \Gamma(\frac{\varepsilon+5}{2}) \Gamma(\frac{\varepsilon}{2}+n+1) \Gamma(-j_1-j_2+n-4)}$$

+  $\sim \mathbf{2400}$  further multi-sums

↓ (see talk)

$$D_\varepsilon(n) = \varepsilon^{-3} F_{-3}(n) + \varepsilon^{-2} F_{-2}(n) + \varepsilon^{-1} F_{-1}(n) + \varepsilon^0 F_0(n) + \dots$$

## General tactic

**Feynman parameter integrals** with one mass  $M$  and local operator insertions in  $4 + \varepsilon$ -dimensional Minkowski space:

$$D_\varepsilon(n) = \int \frac{d^D p_1}{(2\pi)^D} \cdots \int \frac{d^D p_k}{(2\pi)^D} \frac{N(p_1, \dots, p_k; p; M^2; \Delta, n)}{(-p_1^2 + m_1^2)^{l_1} \cdots (-p_k^2 + m_k^2)^{l_k}} \prod_V \delta_V$$

↓ (Blümlein/Stan/Schneider 2012)

**Definite hypergeometric multi-sums:**

$$D_\varepsilon(n) = \sum_{k_1=l_1}^{L_1(n)} \cdots \sum_{k_v=l_v}^{L_v(n, k_1, \dots, k_{v-1})} \sum_{i=1}^l f_i(\varepsilon, n, k_1, \dots, k_v)$$

$f_i$ : proper hypergeometric series in terms of  $\Gamma$ -functions

$L_v(n, k_1, \dots, k_{v-1})$ : integer linear relation in the parameters (or  $\infty$ )

↓ (symbolic summation)

$$D_\varepsilon(n) = \varepsilon^{-3} F_{-3}(n) + \varepsilon^{-2} F_{-2}(n) + \varepsilon^{-1}(n) F_{-1}(n) + \dots$$

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$$\times \frac{(-1)^{j_1} (j_2+1) \Gamma(-\frac{\varepsilon}{2}+j_1+4) \Gamma(-j_1+n-2) \Gamma(\varepsilon-j_1-j_2+n-5)}{(\varepsilon-10)(\varepsilon-8)(\varepsilon-2)\varepsilon \Gamma(\frac{5}{2}-\varepsilon) \Gamma(\frac{\varepsilon+5}{2}) \Gamma(\frac{\varepsilon}{2}+n+1) \Gamma(-j_1-j_2+n-4)}$$

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## Step 1: Expansion of the summand

$$\begin{aligned}
 & \sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \pi 2^{\varepsilon+3} e^{-\frac{3\gamma\varepsilon}{2}} \Gamma(2-\varepsilon) \Gamma\left(\frac{\varepsilon}{2}+2\right) \Gamma\left(-\frac{3\varepsilon}{2}\right) \\
 & \quad \times \underbrace{\frac{(-1)^{j_1}(j_2+1)\Gamma\left(-\frac{\varepsilon}{2}+j_1+4\right)\Gamma(-j_1+n-2)\Gamma(\varepsilon-j_1-j_2+n-5)}{(\varepsilon-10)(\varepsilon-8)(\varepsilon-2)\varepsilon\Gamma\left(\frac{5}{2}-\varepsilon\right)\Gamma\left(\frac{\varepsilon+5}{2}\right)\Gamma\left(\frac{\varepsilon}{2}+n+1\right)\Gamma(-j_1-j_2+n-4)}} \\
 & \quad \varepsilon^{-3} f_{-3}(n, j_2, j_1) + \varepsilon^{-2} f_{-2}(n, j_2, j_1) + \varepsilon^{-1} f_{-1}(n, j_2, j_1) + \dots
 \end{aligned}$$

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$$\sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \pi 2^{\varepsilon+3} e^{-\frac{3\gamma\varepsilon}{2}} \Gamma(2-\varepsilon) \Gamma\left(\frac{\varepsilon}{2}+2\right) \Gamma\left(-\frac{3\varepsilon}{2}\right) \\ \times \underbrace{\frac{(-1)^{j_1} (j_2+1) \Gamma\left(-\frac{\varepsilon}{2}+j_1+4\right) \Gamma(-j_1+n-2) \Gamma(\varepsilon-j_1-j_2+n-5)}{(\varepsilon-10)(\varepsilon-8)(\varepsilon-2)\varepsilon \Gamma\left(\frac{5}{2}-\varepsilon\right) \Gamma\left(\frac{\varepsilon+5}{2}\right) \Gamma\left(\frac{\varepsilon}{2}+n+1\right) \Gamma(-j_1-j_2+n-4)}} \\ \varepsilon^{-3} f_{-3}(n, j_2, j_1) + \varepsilon^{-2} f_{-2}(n, j_2, j_1) + \varepsilon^{-1} f_{-1}(n, j_2, j_1) + \dots$$

$$= \varepsilon^{-3} \boxed{0} + \varepsilon^{-2} \boxed{\sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} f_{-2}(n, j_2, j_1)} + \varepsilon^{-2} \boxed{\sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} f_{-2}(n, j_2, j_1)} \dots$$



## Step 2: Simplify sums from inside to outside

$$\sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \frac{-8(j_1+2)(j_1+3)(n+1)(j_1-n+3)(j_1-n+4)(-1)^{j_1}(j_1+1)!(-j_1+n-5)!(j_2+1)}{135(n+1)!(j_1+j_2-n+5)}$$

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$$\times \left[ \sum_{j_2=0}^{n-j_1-6} \frac{j_2+1}{j_1+j_2-n+5} \right]$$

$$(n + 2)(-j_1 + n - 5)\mathbf{A}(j_1) + (j_1 - n + 4)\mathbf{A}(j_1 + 1) = j_1 - n + 5$$

recurrence finder

$$A(j_1) = \sum_{j_2=0}^{n-j_1-6} \frac{j_2 + 1}{j_1 + j_2 - n + 5}$$

$$(n + 2)(-j_1 + n - 5)\mathbf{A}(j_1) + (j_1 - n + 4)\mathbf{A}(j_1 + 1) = j_1 - n + 5$$

recurrence solver

$$A(j_1) = \sum_{j_2=0}^{n-j_1-6} \frac{j_2 + 1}{j_1 + j_2 - n + 5}$$

∈

$$\left\{ (n - j_1 - 4) \sum_{i=1}^{j_1} \frac{1}{-3 + n - i} + c \times (n - j_1 - 4) \mid c \in \mathbb{R} \right\}$$

$$(n+2)(-j_1+n-5)\mathbf{A}(j_1) + (j_1-n+4)\mathbf{A}(j_1+1) = j_1-n+5$$

## Difference field algorithms/theory

(see, e.g., Karr 1981, Bronstein 2000, Schneider 2001/2004/2005a-c/2007/2008/2010a-c)

$$A(j_1) = \sum_{j_2=0}^{n-j_1-6} \frac{j_2+1}{j_1+j_2-n+5} = (n-j_1-4) \left( \sum_{i=1}^{j_1} \frac{1}{-3+n-i} \right) + \frac{(n^4-2n^3-7n^2+16n-6)}{(n-3)(n-2)(n-1)n} - S_1(n)$$

where

$$S_1(n) = \sum_{i=1}^n \frac{1}{i}$$

# More generally: Sigma's summation spiral

## 1. Creative telescoping (for the special case of hypergeometric terms see Zeilberger's algorithm (1991))

GIVEN a **definite** sum

$$A(n) = \sum_{k=0}^n f(n, k);$$

$f(n, k)$ : indefinite nested product-sum in  $k$ ;  
 $n$ : extra parameter

FIND a **recurrence** for  $A(n)$

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## 2. Recurrence solving

GIVEN a recurrence

$a_0(n), \dots, a_d(n), h(n)$ :  
 indefinite nested product-sum expressions.

$$a_0(n)A(n) + \dots + a_d(n)A(n+d) = h(n);$$

FIND **all solutions** expressible by indefinite nested products and sums  
 (Abramov/Bronstein/Petkovšek/Schneider, in preparation)

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3. Find a "closed form"

$A(n)$ =combined solutions.



## Step 2: Simplify sums from inside to outside

$$\sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \frac{-8(j_1+2)(j_1+3)(n+1)(j_1-n+3)(j_1-n+4)(-1)^{j_1}(j_1+1)!(-j_1+n-5)!(j_2+1)}{135(n+1)!(j_1+j_2-n+5)}$$

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$$\times \left[ \sum_{j_2=0}^{n-j_1-6} \frac{j_2+1}{j_1+j_2-n+5} \right]$$

||

$$(n-j_1-4) \left( \sum_{i=1}^{j_1} \frac{1}{-3+n-i} + \frac{(n^4-2n^3-7n^2+16n-6)}{(n-3)(n-2)(n-1)n} - S_1(n) \right)$$

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 & \quad \parallel \\
 & \sum_{j_1=0}^{n-5} \frac{-8(j_1+2)(j_1+3)(n+1)(j_1-n+3)(j_1-n+4)(-1)^{j_1}(j_1+1)!(-j_1+n-5)!}{135(n+1)!} \times \\
 & \quad \times (n - j_1 - 4) \left( \sum_{i=1}^{j_1} \frac{1}{-3 + n - i} + \frac{(n^4 - 2n^3 - 7n^2 + 16n - 6)}{(n-3)(n-2)(n-1)n} - S_1(n) \right)
 \end{aligned}$$

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$$\parallel$$

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$$\times (n - j_1 - 4) \left( \sum_{i=1}^{j_1} \frac{1}{-3 + n - i} + \frac{(n^4 - 2n^3 - 7n^2 + 16n - 6)}{(n-3)(n-2)(n-1)n} - S_1(n) \right)$$

$$\parallel$$

$$- \frac{16(n^8 + 6n^7 - 6n^6 - 80n^5 - 81n^4 + 178n^3 + 274n^2 - 4n - 96)}{45(n-2)(n-1)^2 n^2 (n+1)(n+2)^2 (n+3)^2}$$

$$+ \frac{16(-1)^n (3n^2 + 12n + 11)}{135(n+1)(n+2)^2 (n+3)^2} + \frac{16(n^2 - n - 8)}{45(n-1)n(n+2)(n+3)} S_1(n)$$

# Mathematica Session:

In[1]:= << **Sigma.m**

Sigma - A summation package by Carsten Schneider © RISC-Linz

In[2]:= << **HarmonicSums.m**

HarmonicSums by Jakob Ablinger © RISC-Linz

In[3]:= << **EvaluateMultiSums.m**

EvaluateMultiSums by Carsten Schneider © RISC-Linz

In[4]:= **EvaluateMultiSum**[

$$\frac{-8(j_1+2)(j_1+3)(n+1)(j_1-n+3)(j_1-n+4)(-1)^{j_1}(j_1+1)!(-j_1+n-5)!(j_2+1)}{135(n+1)!(j_1+j_2-n+5)},$$

{ {j<sub>2</sub>, 0, n - j<sub>1</sub> - 6}, {j<sub>1</sub>, 0, N - 5}}, {n}, {5}, ExpandIn → {ε, -3, -1}]

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$$\frac{-8(j_1+2)(j_1+3)(n+1)(j_1-n+3)(j_1-n+4)(-1)^{j_1}(j_1+1)!(-j_1+n-5)!(j_2+1)}{135(n+1)!(j_1+j_2-n+5)},$$

{ {j<sub>2</sub>, 0, n - j<sub>1</sub> - 6}, {j<sub>1</sub>, 0, N - 5}}, {n}, {5}, **ExpandIn** → {ε, -3, -1}]

$$\text{Out[4]} = \left\{ 0, \frac{16(-1)^n(3n^2+12n+11)}{135(n+1)(n+2)^2(n+3)^2} - \frac{16(n^8+6n^7-6n^6-80n^5-81n^4+178n^3+274n^2-4n-96)}{45(n-2)(n-1)^2n^2(n+1)(n+2)^2(n+3)^2} \right.$$

$$\frac{16(n^2-n-8)}{45(n-1)n(n+2)(n+3)} S_1(n), \quad - \frac{8(n^2-n-8)}{45(n-1)n(n+2)(n+3)} S_2(n) + \frac{2(-1)^n(187n+127)(3n^2+12n+11)}{2025(n+1)^2(n+2)^2(n+3)^2}$$

$$\left. + \left( \frac{2(17n^6-231n^5+121n^4+2063n^3-1458n^2-2432n+960)}{675(n-2)(n-1)^2n^2(n+1)(n+2)(n+3)} - \frac{16(-1)^n(3n^2+12n+11)}{135(n+1)(n+2)^2(n+3)^2} \right) S_1(n) + \right.$$

$$\left. \frac{2(43n^{12}+112n^{11}+263n^{10}-216n^9-11309n^8-16476n^7+55837n^6+78164n^5-95178n^4-116688n^3+51784n^2+30624n-23040)}{675(n-2)^2(n-1)^3n^3(n+1)^2(n+2)^2(n+3)^2} \right\}$$

So far, the most complicated 3-loop ladder graph:



$$= F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \boxed{F_0(n)}$$

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$$\sum_{j=0}^{n-3} \sum_{k=0}^j \sum_{l=0}^k \sum_{q=0}^{-j+n-3-l+n-q-3} \sum_{s=1}^{-l+n-q-3} \sum_{r=0}^{-l+n-q-s-3} (-1)^{-j+k-l+n-q-3} \times$$

$$\times \frac{\binom{j+1}{k+1} \binom{k}{l} \binom{n-1}{j+2} \binom{-j+n-3}{q} \binom{-l+n-q-3}{s} \binom{-l+n-q-s-3}{r} r! (-l+n-q-r-s-3)! (s-1)!}{(-l+n-q-2)! (-j+n-1) (n-q-r-s-2) (q+s+1)}$$

$$\left[ 4S_1(-j+n-1) - 4S_1(-j+n-2) - 2S_1(k) \right.$$

$$\left. - (S_1(-l+n-q-2) + S_1(-l+n-q-r-s-3) - 2S_1(r+s)) \right.$$

$$\left. + 2S_1(s-1) - 2S_1(r+s) \right] + \mathbf{3 \text{ further 6-fold sums}}$$

$$\begin{aligned}
\boxed{F_0(n)} = & \\
& \frac{7}{12} S_1(n)^4 + \frac{(17n+5)S_1(n)^3}{3n(n+1)} + \left( \frac{35n^2-2n-5}{2n^2(n+1)^2} + \frac{13S_2(n)}{2} + \frac{5(-1)^n}{2n^2} \right) S_1(n)^2 \\
& + \left( -\frac{4(13n+5)}{n^2(n+1)^2} + \left( \frac{4(-1)^n(2n+1)}{n(n+1)} - \frac{13}{n} \right) S_2(n) + \left( \frac{29}{3} - (-1)^n \right) S_3(n) \right. \\
& + \left( 2 + 2(-1)^n \right) S_{2,1}(n) - 28S_{-2,1}(n) + \frac{20(-1)^n}{n^2(n+1)} \left. \right) S_1(n) + \left( \frac{3}{4} + (-1)^n \right) S_2(n)^2 \\
& - 2(-1)^n S_{-2}(n)^2 + S_{-3}(n) \left( \frac{2(3n-5)}{n(n+1)} + (26 + 4(-1)^n) S_1(n) + \frac{4(-1)^n}{n+1} \right) \\
& + \left( \frac{(-1)^n(5-3n)}{2n^2(n+1)} - \frac{5}{2n^2} \right) S_2(n) + S_{-2}(n) \left( 10S_1(n)^2 + \frac{8(-1)^n(2n+1)}{n(n+1)} \right. \\
& + \left. \frac{4(3n-1)}{n(n+1)} \right) S_1(n) + \frac{8(-1)^n(3n+1)}{n(n+1)^2} + \left( -22 + 6(-1)^n \right) S_2(n) - \frac{16}{n(n+1)} \\
& + \left( \frac{(-1)^n(9n+5)}{n(n+1)} - \frac{29}{3n} \right) S_3(n) + \left( \frac{19}{2} - 2(-1)^n \right) S_4(n) + \left( -6 + 5(-1)^n \right) S_{-4}(n) \\
& + \left( -\frac{2(-1)^n(9n+5)}{n(n+1)} - \frac{2}{n} \right) S_{2,1}(n) + (20 + 2(-1)^n) S_{2,-2}(n) + (-17 + 13(-1)^n) S_{3,1}(n) \\
& - \frac{8(-1)^n(2n+1) + 4(9n+1)}{n(n+1)} S_{-2,1}(n) - (24 + 4(-1)^n) S_{-3,1}(n) + (3 - 5(-1)^n) S_{2,1,1}(n) \\
& + 32S_{-2,1,1}(n) + \left( \frac{3}{2} S_1(n)^2 - \frac{3S_1(n)}{n} + \frac{3}{2} (-1)^n S_{-2}(n) \right) \zeta(2)
\end{aligned}$$



## Strategies 2,3,4: Find a recurrence for the integral/sum

$$D_\varepsilon(n) = \int_0^1 \dots \int_0^1 \Phi(\varepsilon, n, x_1, x_2, \dots, x_7) dx_1 dx_2 \dots dx_7$$
$$\stackrel{?}{=} F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \dots$$

multivariate  
Almquist/Zeilberger  
(Jakob Ablinger)

$$a_0(\varepsilon, n)D_\varepsilon(n) + \dots + a_d(\varepsilon, n)D_\varepsilon(n + d) = h(\varepsilon, n)$$

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$$\sum_{i_1} \dots \sum_{i_7} f(\varepsilon, n, i_1, i_2, \dots, i_7)$$

MultiSum Package  
(Flavia Stan)

$$a_0(\varepsilon, n)D_\varepsilon(n) + \dots + a_d(\varepsilon, n)D_\varepsilon(n + d) = h(\varepsilon, n)$$

## Strategies 2,3,4: Find a recurrence for the integral/sum

$$D_\varepsilon(n) = \int_0^1 \dots \int_0^1 \Phi(\varepsilon, n, x_1, x_2, \dots, x_7) dx_1 dx_2 \dots dx_7$$

$$\stackrel{?}{=} F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \dots$$

multivariate  
Almquist/Zeilberger  
(Jakob Ablinger)

$$\sum_{i_1} \dots \sum_{i_7} f(\varepsilon, n, i_1, i_2, \dots, i_7)$$

MultiSum Package  
(Flavia Stan)

Holonomic/difference field Approach  
(Mark Round)

$$a_0(\varepsilon, n)D_\varepsilon(n) + \dots + a_d(\varepsilon, n)D_\varepsilon(n+d) = h(\varepsilon, n)$$

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 $\varepsilon$ -recurrence solver

multivariate  
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$$a_0(\varepsilon, n)D_\varepsilon(n) + \dots + a_d(\varepsilon, n)D_\varepsilon(n+d) = h(\varepsilon, n)$$

## Ansatz (for power series)

$$\begin{aligned}
 & a_0(\varepsilon, n) \left[ F_0(n) + F_1(n)\varepsilon + F_2(n)\varepsilon^2 + \dots \right] \\
 & + a_1(\varepsilon, n) \left[ F_0(n+1) + F_1(n+1)\varepsilon + F_2(n+1)\varepsilon^2 + \dots \right] \\
 & + \\
 & \vdots \\
 & + a_d(\varepsilon, n) \left[ F_0(n+d) + F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\
 & \qquad \qquad \qquad = h_0(n) + h_1(n)\varepsilon + h_1(n)\varepsilon^2 + \dots
 \end{aligned}$$



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 & + \\
 & \vdots \\
 & + a_d(\varepsilon, n) \left[ F_0(n+d) + F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\
 & \qquad \qquad \qquad = h_0(n) + h_1(n)\varepsilon + h_1(n)\varepsilon^2 + \dots
 \end{aligned}$$

↓ constant terms must agree

$$a_0(0, n)F_0(n) + a_1(n)F_0(n+1) + \dots + a_d(n)F_0(n+d) = h_0(n)$$

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 & + \\
 & \vdots \\
 & + a_d(\varepsilon, n) \left[ F_0(n+d) + F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\
 & \qquad \qquad \qquad = h_0(n) + h_1(n)\varepsilon + h_1(n)\varepsilon^2 + \dots
 \end{aligned}$$

⇓ constant terms must agree

$$a_0(0, n)F_0(n) + a_1(n)F_0(n+1) + \dots + a_d(n)F_0(n+d) = h_0(n)$$

If  $F_0(n)$  (with required initial values) is not expressible in terms of indefinite nested sums and products:

**game over**

## Ansatz (for power series)

$$\begin{aligned}
 & a_0(\varepsilon, n) \left[ F_0(n) + F_1(n)\varepsilon + F_2(n)\varepsilon^2 + \dots \right] \\
 & + a_1(\varepsilon, n) \left[ F_0(n+1) + F_1(n+1)\varepsilon + F_2(n+1)\varepsilon^2 + \dots \right] \\
 & + \\
 & \vdots \\
 & + a_d(\varepsilon, n) \left[ F_0(n+d) + F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\
 & \qquad \qquad \qquad = h_0(n) + h_1(n)\varepsilon + h_1(n)\varepsilon^2 + \dots
 \end{aligned}$$

⇓ constant terms must agree

$$a_0(0, n)F_0(n) + a_1(n)F_0(n+1) + \dots + a_d(n)F_0(n+d) = h_0(n)$$



## Ansatz (for power series)

$$\begin{aligned}
 & a_0(\varepsilon, n) \left[ F_0(n) + F_1(n)\varepsilon + F_2(n)\varepsilon^2 + \dots \right] \\
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 & + \\
 & \vdots \\
 & + a_d(\varepsilon, n) \left[ F_0(n+d) + F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\
 & \qquad \qquad \qquad = h_0(n) + h_1(n)\varepsilon + h_1(n)\varepsilon^2 + \dots
 \end{aligned}$$

↓ constant terms must agree

$$a_0(0, n)F_0(n) + a_1(n)F_0(n+1) + \dots + a_d(n)F_0(n+d) = h_0(n)$$

$$\begin{aligned} & a_0(\varepsilon, n) \left[ F_1(n)\varepsilon + F_2(n)\varepsilon^2 + \dots \right] \\ & + a_1(\varepsilon, n) \left[ F_1(n+1)\varepsilon + F_2(n+1)\varepsilon^2 + \dots \right] \\ & + \\ & \vdots \\ & + a_d(\varepsilon, n) \left[ F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\ & = h'_0(n) + h'_1(n)\varepsilon + h'_2(n)\varepsilon^2 + \dots \end{aligned}$$

$$\begin{aligned}
 & a_0(\varepsilon, n) \left[ F_1(n)\varepsilon + F_2(n)\varepsilon^2 + \dots \right] \\
 & + a_1(\varepsilon, n) \left[ F_1(n+1)\varepsilon + F_2(n+1)\varepsilon^2 + \dots \right] \\
 & + \\
 & \vdots \\
 & + a_d(\varepsilon, n) \left[ F_1(n+d)\varepsilon + F_2(n+d)\varepsilon^2 + \dots \right] \\
 & \qquad \qquad \qquad = \underbrace{h'_0(n) + h'_1(n)}_{=0} \varepsilon + h'_2(n)\varepsilon^2 + \dots
 \end{aligned}$$

Divide by  $\varepsilon$

$$\begin{aligned} & a_0(\varepsilon, n) \left[ F_1(n) + F_2(n)\varepsilon + \dots \right] \\ & + a_1(\varepsilon, n) \left[ F_1(n+1) + F_2(n+1)\varepsilon + \dots \right] \\ & + \\ & \vdots \\ & + a_d(\varepsilon, n) \left[ F_1(n+d) + F_2(n+d)\varepsilon + \dots \right] = h'_1(n) + h'_2(n)\varepsilon + \dots \end{aligned}$$

**Now repeat for**  $F_1(n), F_2(n), \dots$

Remark: Works the same for Laurent series.

For math/CA details: J. Symbolic Comput. 2012 [arXiv:1011.2656v1]

# Computer algebra and special functions:

**Harmonic sums** (J. Vermaseren, J. Blümlein; M. Hoffman, D. Broadhurst, . . . )

$$S_{2,1}(n) = \sum_{i=1}^n \frac{1}{i^2} \sum_{j=1}^i \frac{1}{j}$$

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$$S_{2,1}(n) = \sum_{i=1}^n \frac{1}{i^2} \sum_{j=1}^i \frac{1}{j}$$

**Integral representation:**

$$= \int_0^1 \frac{x^n - 1}{1-x} \left( \int_0^x \frac{\int_0^y \frac{1}{1-z} dz}{y} dy - \zeta(2) \right) dx,$$

$$\zeta(z) := \sum_{i=1}^{\infty} 1/i^z$$

# Computer algebra and special functions:

**Harmonic sums** (J. Vermaseren, J. Blümlein; M. Hoffman, D. Broadhurst, ...)

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**Asymptotic expansion:**

$$= \left( \frac{1}{30n^5} - \frac{1}{6n^3} + \frac{1}{2n^2} - \frac{1}{n} \right) \ln(n) \\ - \frac{1}{100n^5} - \frac{1}{6n^4} + \frac{13}{36n^3} - \frac{1}{4n^2} - \frac{1}{n} + 2\zeta(3) + O\left(\frac{\ln(n)}{n^6}\right).$$

**limit computations**

**numerical evaluation**

# Computer algebra and special functions:

**Generalization to cyclotomic harmonic sums** (J. Ablinger, J. Blümlein, CS)

$$\boxed{\sum_{k=1}^n \frac{(-1)^k}{2k+1}} =$$

**Integral representation:**

$$= -(-1)^n \int_0^1 \frac{x^{2n}}{x^2+1} dx + \frac{(-1)^n}{2n+1} - 1 + \frac{\pi}{4},$$

**Asymptotic expansion:**

$$= (-1)^n \left( -\frac{3}{64n^5} - \frac{1}{16n^4} + \frac{3}{16n^3} - \frac{1}{4n^2} + \frac{1}{4n} \right) + \frac{\pi}{4} - 1 + O\left(\frac{1}{n^6}\right)$$

**limit computations**

**numerical evaluation**



$$\sum_{i=1}^n \frac{\sum_{j=1}^i \frac{1}{j^2}}{(2i+1)^2} = \text{asymptotic expansion?}$$

In[5]:= << **HarmonicSums.m**

HarmonicSums by Jakob Ablinger © RISC-Linz

In[6]:= **SExpansion[S[{{2, 1, 2}, {1, 0, 2}}, n], n, 10]**

$$\sum_{i=1}^n \frac{\sum_{j=1}^i \frac{1}{j^2}}{(2i+1)^2} = \text{asymptotic expansion?}$$

In[5]:= << HarmonicSums.m

HarmonicSums by Jakob Ablinger © RISC-Linz

In[6]:= SExpansion[S[{{2, 1, 2}, {1, 0, 2}}, n], n, 10]

$$\begin{aligned} \text{Out}[6]= & \left( -\frac{16\ln^2 2}{3} + \frac{3}{128n^{10}} - \frac{367}{5760n^9} + \frac{7}{96n^8} - \frac{221}{2016n^7} + \frac{5}{24n^6} - \frac{127}{360n^5} + \frac{1}{2n^4} - \frac{11}{18n^3} + \right. \\ & \left. \frac{2}{3n^2} - \frac{2}{3n} - \frac{1936}{15} \right) \frac{1}{4} (\pi - 4)^2 + \left( -\frac{32\ln^2 2}{3} + \frac{3}{64n^{10}} - \frac{367}{2880n^9} + \frac{7}{48n^8} - \frac{221}{1008n^7} + \right. \\ & \left. \frac{5}{12n^6} - \frac{127}{180n^5} + \frac{1}{n^4} - \frac{11}{9n^3} + \frac{4}{3n^2} - \frac{4}{3n} - \frac{3872}{45} \right) \frac{1}{4} (\pi - 4) - \frac{968}{45} \frac{1}{4} (\pi - 4)^4 - \\ & \frac{3872}{45} \frac{1}{4} (\pi - 4)^3 + 8\text{li4half} + \frac{\ln^2 4}{3} - \frac{16\ln^2 2}{3} + 7\ln 2 z^3 + \frac{125891}{1075200n^{10}} - \frac{10259}{80640n^9} + \\ & \frac{92257}{645120n^8} - \frac{5507}{20160n^7} + \frac{2837}{5760n^6} - \frac{509}{720n^5} + \frac{161}{192n^4} - \frac{31}{36n^3} + \frac{19}{24n^2} - \frac{2}{3n} - \frac{968}{45} \end{aligned}$$

# Example: 3-loop topologies of gluonic massive operator matrix elements with two fermion lines (unpolarized case)

$$D_\varepsilon(n) = \text{[diagram 1]} + \text{[diagram 2]} + \sim \mathbf{80 \text{ further diagrams}}$$

[by axodraw (J. Vermaseren)]

↓ J. Blümlein, A. Hasselhuhn

$$D_\varepsilon(n) = \sum_{j_1=0}^{n-5} \sum_{j_2=0}^{n-j_1-6} \pi^2 \varepsilon^{+3} e^{-\frac{3\gamma\varepsilon}{2}} \Gamma(2-\varepsilon) \Gamma\left(\frac{\varepsilon}{2}+2\right) \Gamma\left(-\frac{3\varepsilon}{2}\right) \quad (\sim 2\text{GB})$$

$$\times \frac{(-1)^{j_1} (j_2+1) \Gamma(-\frac{\varepsilon}{2}+j_1+4) \Gamma(-j_1+n-2) \Gamma(\varepsilon-j_1-j_2+n-5)}{(\varepsilon-10)(\varepsilon-8)(\varepsilon-2)\varepsilon \Gamma(\frac{5}{2}-\varepsilon) \Gamma(\frac{\varepsilon+5}{2}) \Gamma(\frac{\varepsilon}{2}+n+1) \Gamma(-j_1-j_2+n-4)}$$

+  $\sim \mathbf{2400}$  further multi-sums

↓ **time:  $\sim 8$  month**

$$D_\varepsilon(n) = \varepsilon^{-3} F_{-3}(n) + \varepsilon^{-2} F_{-2}(n) + \varepsilon^{-1} F_{-1}(n) + \varepsilon^0 F_0(n) + \dots$$

# Efficient calculation

## 1. Reduction to key sums

- Synchronize 2400 sums to 4 sums:

$$\sum_{i_2=5}^{n-5} \sum_{i_1=0}^{i_2} h_1(\varepsilon, n, i_2, i_1)$$

$$\sum_{i_2=0}^{n-5} \sum_{i_1=0}^{n-i_2-5} h_2(\varepsilon, n, i_2, i_1)$$

$$\sum_{i_1=5}^{n-5} h_3(\varepsilon, n, i_1)$$

$$\sum_{i_1=0}^{\infty} h_4(\varepsilon, n, i_1)$$

**Note: 4 sums plus sum-free expression > 2 GB**

# Efficient calculation

## 1. Reduction to key sums

- ▶ Synchronize 2400 sums to 4 sums:

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$$\sum_{i_2=0}^{n-5} \sum_{i_1=0}^{n-i_2-5} h_2(\varepsilon, n, i_2, i_1)$$

$$\sum_{i_1=5}^{n-5} h_3(\varepsilon, n, i_1)$$

$$\sum_{i_1=0}^{\infty} h_4(\varepsilon, n, i_1)$$

**Note: 4 sums plus sum-free expression > 2 GB**

- ▶ Eliminate algebraic relations among  $\Gamma$ /Pochhammer/binomial symbols

## Efficient calculation

### 1. Reduction to key sums

- ▶ Synchronize 2400 sums to 4 sums:

$$\sum_{i_2=5}^{n-5} \sum_{i_1=0}^{i_2} h_1(\varepsilon, n, i_2, i_1)$$

$$\sum_{i_2=0}^{n-5} \sum_{i_1=0}^{n-i_2-5} h_2(\varepsilon, n, i_2, i_1)$$

$$\sum_{i_1=5}^{n-5} h_3(\varepsilon, n, i_1)$$

$$\sum_{i_1=0}^{\infty} h_4(\varepsilon, n, i_1)$$

**Note: 4 sums plus sum-free expression > 2 GB**

- ▶ Eliminate algebraic relations among  $\Gamma$ /Pochhammer/binomial symbols
- ▶ Write the sums in the form

$$\sum (\text{product of } \Gamma/\text{Pochhammer/binomial symbols}) * (\text{rational function})$$

**Note: 29 sums, total size: 7.6 MB**

# Efficient calculation

## 1. Reduction to key sums

```
In[7]:= << SumProduction.m
```

SumProduction - A summation package by Carsten Schneider © RISC-Linz

```
In[8]:= expr = << DESYInput.txt;
```

```
In[9]:= compactExpr =
```

```
ReduceMultiSums[expr, {n}, {5}];
```

7hours

2GB → 7.6MB

## Efficient calculation

### 1. Reduction to key sums

In[7]:= << **SumProduction.m**

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In[8]:= **expr =**<<< **DESYInput.txt**;

In[9]:= **compactExpr =**

**ReduceMultiSums[expr, {n}, {5}];**

7hours

2GB → 7.6MB

### 2. (Parallel) calculation of the $\varepsilon$ -expansion for each sum:

In[10]:= **ProcessEachSum[compactExpr, {n}, {6},**

**ExpandIn → {ep, -3, 0}]**

90minutes



## Efficient calculation

### 1. Reduction to key sums

In[7]:= << SumProduction.m

SumProduction - A summation package by Carsten Schneider © RISC-Linz

In[8]:= expr = << DESYInput.txt;

In[9]:= compactExpr =

ReduceMultiSums[expr, {n}, {5}];

7hours

2GB → 7.6MB

### 2. (Parallel) calculation of the $\varepsilon$ -expansion for each sum:

In[10]:= ProcessEachSum[compactExpr, {n}, {6},

ExpandIn → {ep, -3, 0}]

90minutes

### 3. Combine expansions (+eliminate algebraic relations):

In[11]:= CombineExpression[compactExpr, {n}, {6}];

20seconds

7.6MB → 0.1MB

# Example: 3-loop topologies of gluonic massive operator matrix elements with two fermion lines (unpolarized case)

$$D_\varepsilon(n) = \text{[by axodraw (J. Vermaseren)]} + \text{[diagram]} + \boxed{\sim 80 \text{ further diagrams}}$$

$$\varepsilon^{-3} F_{-3}(n) + \varepsilon^{-2} F_{-2}(n) + \varepsilon^{-1} F_{-1}(n) + \varepsilon^0 F_0(n) + \dots$$

where

$$F_{-3} = C_A \left( \frac{512}{27} S_1(n) - \frac{64(3n^4 + 6n^3 + 19n^2 + 28n + 28)}{27(n-1)n(n+1)(n+2)} \right) - \frac{512C_F(n^2 + n + 2)^2}{9(n-1)n^2(n+1)^2(n+2)}$$

$$F_{-2} = C_A \left( \frac{64(20n^2 - 20n + 9)S_1(n)}{81(n-1)n} - \frac{16(3n^6 + 9n^5 + 367n^4 + 839n^3 + 1046n^2 + 568n + 96)}{81(n-1)n^2(n+1)^2(n+2)} \right) \\ + C_F \left( \frac{128(n^2 + n + 2)^2 S_1(n)}{9(n-1)n^2(n+1)^2(n+2)} - \frac{128(14n^6 + 33n^5 + 59n^4 + 39n^3 + 55n^2 + 20n - 12)}{27(n-1)n^3(n+1)^3(n+2)} \right)$$

$$F_{-1} = C_A \left( \zeta_2 \left( \frac{64}{9} S_1(n) - \frac{8(3n^4 + 6n^3 + 19n^2 + 28n + 28)}{9(n-1)n(n+1)(n+2)} \right) + \frac{64(20n^6 + 57n^5 + 12n^4 - 56n^3 - 61n^2 - 30n - 16)S_1(n)}{27(n-1)n^2(n+1)^2(n+2)} \right. \\ \left. - \frac{4(57n^8 + 228n^7 + 4044n^6 + 12486n^5 + 17787n^4 + 12342n^3 + 1952n^2 - 2368n - 960)}{81(n-1)n^3(n+1)^3(n+2)} \right) \\ + C_F \left( - \frac{160(n^2 + n + 2)^2 S_1(n)^2}{9(n-1)n^2(n+1)^2(n+2)} + \frac{32(n^2 + n + 2)^2 S_2(n)}{3(n-1)n^2(n+1)^2(n+2)} + \frac{64(16n^6 + 57n^5 + 268n^4 + 465n^3 + 410n^2 + 208n + 4)}{27(n-1)n^3(n+1)^3(n+2)} \right. \\ \left. - \frac{64(n^2 + n + 2)^2 \zeta_2}{3(n-1)n^2(n+1)^2(n+2)} - \frac{64(185n^8 + 704n^7 + 1712n^6 + 2699n^5 + 3694n^4 + 3801n^3 + 2249n^2 + 744n + 180)}{81(n-1)n^4(n+1)^4(n+2)} \right)$$

$$\begin{aligned}
F_0 = & C_A \left( \frac{8S_1(n)^3}{27(n-1)n} + \frac{4(16n^5+31n^4-38n^3-3n^2+50n+32)S_1(n)^2}{27(n-1)n^2(n+1)^2(n+2)} + \left( \frac{8(6944n^8+26480n^7+24941n^6-7003n^5-247}{729(n-1)n^3(n+1)^3(n+2)} \right. \right. \\
& + \frac{8S_2(n)}{9(n-1)n} \Big) S_1(n) + \frac{4809n^{10}+24045n^9-224384n^8-1104398n^7-2105327n^6-2139551n^5-1133210n^4-209408n^3-}{729(n-1)n^4(n+1)^4(n+2)} \\
& + \zeta_3 \left( \frac{56(3n^4+6n^3+19n^2+28n+28)}{27(n-1)n(n+1)(n+2)} - \frac{448}{27} S_1(n) \right) + \zeta_2 \left( \frac{8(20n^2-20n+9)S_1(n)}{27(n-1)n} \right. \\
& - \left. \frac{2(3n^6+9n^5+367n^4+839n^3+1046n^2+568n+96)}{27(n-1)n^2(n+1)^2(n+2)} \right) - \frac{4(40n^6+112n^5+7n^4-126n^3-251n^2-190n-96)S_2(n)}{27(n-1)n^2(n+1)^2(n+2)} + \frac{44}{9(n-1)} \\
& + C_F \left( \frac{112(n^2+n+2)^2 S_1(n)^3}{27(n-1)n^2(n+1)^2(n+2)} - \frac{16(44n^6+123n^5+386n^4+543n^3+520n^2+248n+24)S_1(n)^2}{27(n-1)n^3(n+1)^3(n+2)} \right. \\
& + \left. \left( \frac{16S_2(n)(n^2+n+2)^2}{3(n-1)n^2(n+1)^2(n+2)} + \frac{32(205n^8+856n^7+3169n^6+6484n^5+7310n^4+4722n^3+1534n^2+48n-72)}{81(n-1)n^4(n+1)^4(n+2)} \right) S_1(n) \right. \\
& - \left. \frac{32(1976n^{10}+9385n^9+24088n^8+38989n^7+50214n^6+53872n^5+35219n^4+6890n^3-4233n^2-2844n-756)}{243(n-1)n^5(n+1)^5(n+2)} + \frac{44}{9(n-1)} \right. \\
& - \left. \frac{16(14n^6+33n^5+59n^4+39n^3+55n^2+20n-12)}{9(n-1)n^3(n+1)^3(n+2)} \right) + \frac{16(4n^6+3n^5-50n^4-129n^3-100n^2-56n-24)S_2(n)}{9(n-1)n^3(n+1)^3(n+2)} - \frac{160}{27(n-1)}
\end{aligned}$$

## SUMMARY:

- ▶ Required time: 9 1/2 hours.
- ▶ Occuring sums (after reduction):

$$\zeta_2, \zeta_3, (-1)^n, S_1(n), S_2(n), S_3(n), S_{2,1}(n), S_{3,1}(n), S_{2,1,1}(n).$$

$$\begin{aligned}
F_0 = & C_A \left( \frac{8S_1(n)^3}{27(n-1)n} + \frac{4(16n^5+31n^4-38n^3-3n^2+50n+32)S_1(n)^2}{27(n-1)n^2(n+1)^2(n+2)} + \left( \frac{8(6944n^8+26480n^7+24941n^6-7003n^5-247}{729(n-1)n^3(n+1)^3(n+2)} \right. \right. \\
& + \left. \frac{8S_2(n)}{9(n-1)n} \right) S_1(n) + \frac{4809n^{10}+24045n^9-224384n^8-1104398n^7-2105327n^6-2139551n^5-1133210n^4-209408n^3-}{729(n-1)n^4(n+1)^4(n+2)} \\
& + \zeta_3 \left( \frac{56(3n^4+6n^3+19n^2+28n+28)}{27(n-1)n(n+1)(n+2)} - \frac{448}{27} S_1(n) \right) + \zeta_2 \left( \frac{8(20n^2-20n+9)S_1(n)}{27(n-1)n} \right. \\
& - \left. \frac{2(3n^6+9n^5+367n^4+839n^3+1046n^2+568n+96)}{27(n-1)n^2(n+1)^2(n+2)} \right) - \frac{4(40n^6+112n^5+7n^4-126n^3-251n^2-190n-96)S_2(n)}{27(n-1)n^2(n+1)^2(n+2)} + \frac{44}{9(n-1)} \\
& + C_F \left( \frac{112(n^2+n+2)^2 S_1(n)^3}{27(n-1)n^2(n+1)^2(n+2)} - \frac{16(44n^6+123n^5+386n^4+543n^3+520n^2+248n+24)S_1(n)^2}{27(n-1)n^3(n+1)^3(n+2)} \right. \\
& + \left. \left( \frac{16S_2(n)(n^2+n+2)^2}{3(n-1)n^2(n+1)^2(n+2)} + \frac{32(205n^8+856n^7+3169n^6+6484n^5+7310n^4+4722n^3+1534n^2+48n-72)}{81(n-1)n^4(n+1)^4(n+2)} \right) S_1(n) \right. \\
& - \left. \frac{32(1976n^{10}+9385n^9+24088n^8+38989n^7+50214n^6+53872n^5+35219n^4+6890n^3-4233n^2-2844n-756)}{243(n-1)n^5(n+1)^5(n+2)} + \frac{44}{9(n-1)} \right. \\
& - \left. \frac{16(14n^6+33n^5+59n^4+39n^3+55n^2+20n-12)}{9(n-1)n^3(n+1)^3(n+2)} \right) + \frac{16(4n^6+3n^5-50n^4-129n^3-100n^2-56n-24)S_2(n)}{9(n-1)n^3(n+1)^3(n+2)} - \frac{160}{27(n-1)}
\end{aligned}$$

## SUMMARY:

- ▶ Required time: 9 1/2 hours.
- ▶ Occuring sums (after reduction):

$$\zeta_2, \zeta_3, (-1)^n, S_1(n), S_2(n), S_3(n), S_{2,1}(n), S_{3,1}(n), S_{2,1,1}(n).$$

- ▶ Polarized case has been solved similarly.

$$\begin{aligned}
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- ▶ Polarized case has been solved similarly.
- ▶ For another problem about 100000 triple sums have been reduced to 40 key sums and have been calculated afterwards.

Conclusion:

Integration, Summation and Special Functions  
are important technologies  
in Quantum Field Theory

## LHCPhenoNet School 2012

# Integration, Summation and Special Functions in Quantum Field Theory

Time: July 9 (Mo) to July 13 (Fr)  
Place: RISC, Hagenberg (close to Linz), Upper Austria  
Organizers: J. Blümlein, C. Schneider



# Speakers

## Particle physics



### Special functions

- J. Blümlein (cyclotomic  $\Sigma f$ )
- D. Broadhurst (HPL, H-sums,  $\zeta$ )
- N. Glover (hg. fu in physics)
- D. Kreimer ( $f$ , singularities)
- T. Kornwinder (orthogonal poly)
- P. Paule (survey on hg. fu)
- M. Schlosser (multi-hg. fu)
- S. Weinzierl (graphs)

### Computer algebra

- B. Buchberger (key talk)
- F. Chyzak (holonomic  $\Sigma f$ )
- J. Gerhard (gcd, factorization)
- M. Kauers (guessing)
- O. Pawlyk (hg./asympt. in MMA)
- M. Petkovsek (recurrences)
- C. Raab (Risch's  $f$ )
- C. Schneider ( $\Sigma$ )