

# A numerical approach to NNLO calculations in QCD

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# Outline

- Introduction
- The method
  - simple example
  - multi-loop integrals
  - phase space integrals
  - mixture one loop + single unresolved
- Summary and outlook

## Introduction

Do we need NNLO ?

number of processes/observables where (NLO) theory error dominates (or will dominate at LC)

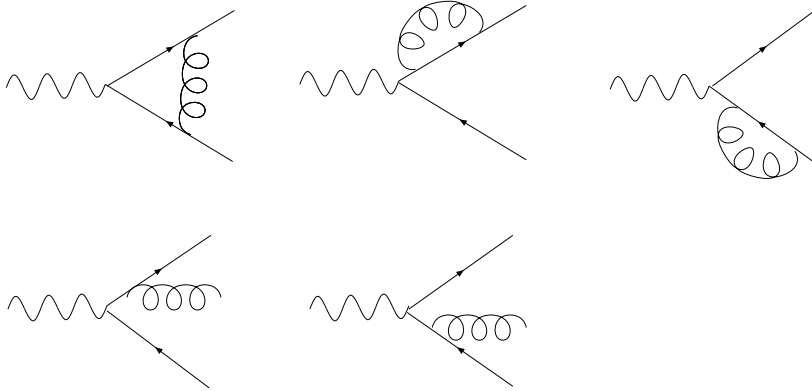
→ see S. Dittmaier's talk

some pro-NNLO arguments:

- reduction of scale dependence
- better modeling of jets
- better description of "intrinsic  $k_T$ " in hadronic initial state
- improved PDF's
- ...
- better understanding of infrared structure of QCD

”conventional” procedure to calculate partonic cross sections:

example NLO:  $\sigma^{NLO} = \underbrace{\sigma^V}_{\text{infinite}} + \underbrace{\sigma^R}_{\text{infinite}}$

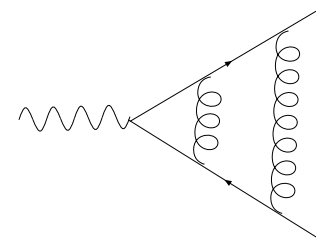


virtual:  $\sum_{i=0}^2 P_i/\epsilon^i$       real: subtraction of  $d\sigma^S$

$$\sigma^{NLO} = \underbrace{\int_{m+1} [d\sigma^R - d\sigma^S]_{\epsilon=0}}_{\text{numerically}} + \underbrace{\int_m \left[ \underbrace{d\sigma^V}_{\text{analytically}} + \underbrace{\int_1 d\sigma^S}_{\text{analytically}} \right]_{\epsilon=0}}_{\text{numerically}}$$

## NNLO: example $e^+e^- \rightarrow 2\text{jets}$

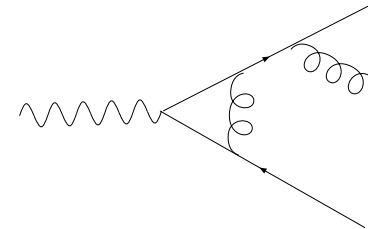
- 2-loop virtual



→ 2-particle phase space

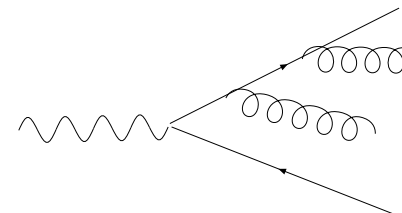
- one-loop single real emission

→ phase space: 1 unresolved particle

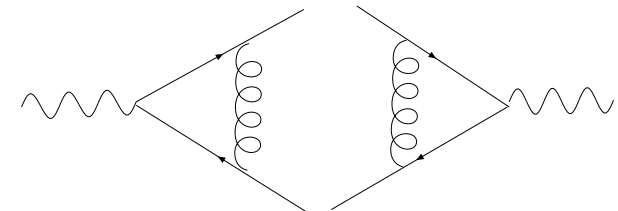


- double real emission

→ difficult phase space integrals:  
up to two unresolved particles



- squares of one-loop amplitudes



problems at NNLO (in "conventional" approach):

- find appropriate subtraction terms
- analytical integration of subtraction terms in  $D = 4 - 2\epsilon$  dimensions  
[see work of A. Gehrmann-De Ridder, T. Gehrmann, N. Glover,  
W. Kilgore, D. A. Kosower, S. Weinzierl]

problem in general:

- construction of a stable and fast Monte Carlo program

main problem in perturbative QCD:

infrared (soft and collinear) divergences:

overlapping structure

example (in parameter space, using dimensional regularization):

$$\int_0^1 dx_1 dx_2 x_1^{-1-\epsilon} [x_1 + x_2]^{-1}$$

occurrence:

multi-loop integrals, phase space integrals, combinations

possible solution:

sector decomposition

# History

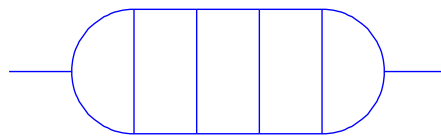
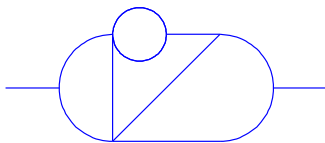
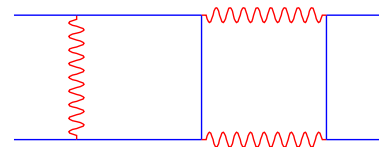
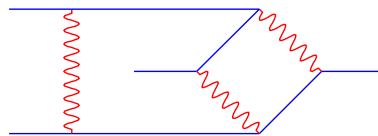
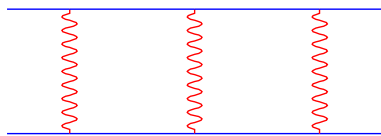
- K. Hepp [Commun. Math. Phys. 2 (1966)]: for overlapping UV divergences
- M. Roth and A. Denner [Nucl. Phys. B 479 (1996)]: high-energy approximation of one-loop Feynman integrals

- iterative, automated algorithm for multi-loop integrals:

T. Binoth, G.H. [Nucl. Phys. B 585 (2000)]

- applied to two-loop box diagrams, massless 3-loop box, 2-point functions up to 5 loops

T. Binoth, G.H. [Nucl. Phys. B 680 (2004)]





application to phase space integrals:

- G.H., Nucl. Phys. Proc. Suppl. 116 (2003)  
(loops & legs 2002)
- A. Gehrmann-De Ridder, T. Gehrmann and G.H., hep-ph/0311276  
all master phase space integrals for  $1 \rightarrow 4$  processes
- C. Anastasiou, K. Melnikov and F. Petriello, hep-ph/0311311  
inclusion of jet function,  $N_f$ -part of  $e^+e^- \rightarrow 2, 3, 4$  jets at  $\mathcal{O}(\alpha_s^2)$
- T. Binoth and G.H., hep-ph/0402265  
partial results for  $e^+e^- \rightarrow 2$  jets
- C. Anastasiou, K. Melnikov and F. Petriello, hep-ph/0402280  
 $e^+e^- \rightarrow 2$  jets

# The Method

simple idea:

$$\begin{aligned} I &= \int_0^\infty dx_1 dx_2 x_1^{-1-\epsilon} (x_1 + x_2)^{-1} \\ &= \int_0^\infty dx_1 dx_2 x_1^{-1-\epsilon} (x_1 + x_2)^{-1} \left[ \underbrace{\Theta(x_1 - x_2)}_{(1)} + \underbrace{\Theta(x_2 - x_1)}_{(2)} \right] \end{aligned}$$

subst. (1)  $x_2 = x_1 t_2$       (2)  $x_1 = x_2 t_1$

$$\begin{aligned} I &= \int_0^\infty dx_1 x_1^{-1-\epsilon} \int_0^1 dt_2 (1 + t_2)^{-1} \\ &\quad + \int_0^\infty dx_2 x_2^{-1-\epsilon} \int_0^1 dt_1 t_1^{-1-\epsilon} (1 + t_1)^{-1} \end{aligned}$$

for more complicated functions one decomposition is not enough  $\Rightarrow$  **iterate**

## Multi-loop integrals:

Input:  $L$ -loop integral with  $N$  propagators after integration over loop momenta

$$G = (-1)^N \Gamma(N - LD/2) \int_0^\infty \prod_{l=1}^N dx_l \delta(1 - \sum_{i=1}^N x_i) \frac{\mathcal{U}(\vec{x})^{N-(L+1)D/2}}{\mathcal{F}(\vec{x}, \{s, m^2\})^{N-LD/2}}$$

example: on-shell massless 2-loop box

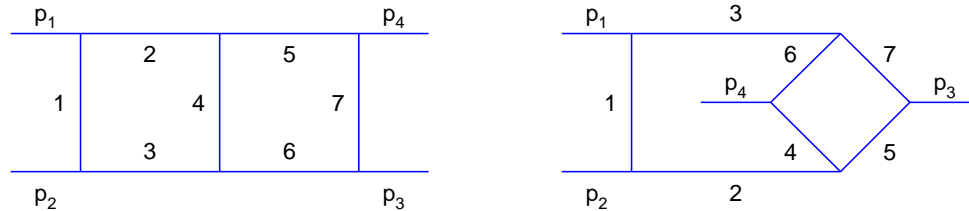
$$G = -\Gamma(3 + 2\epsilon) \int_0^\infty \prod_{l=1}^7 dx_l \delta(1 - \sum_{i=1}^7 x_i) \frac{\mathcal{U}^{1+3\epsilon}}{\mathcal{F}^{3+2\epsilon}}$$

$$\begin{aligned} \mathcal{U} &= (x_1 + x_2 + x_3)(x_5 + x_6 + x_7) \\ &\quad + x_4(x_1 + x_2 + x_3 + x_5 + x_6 + x_7) \end{aligned}$$

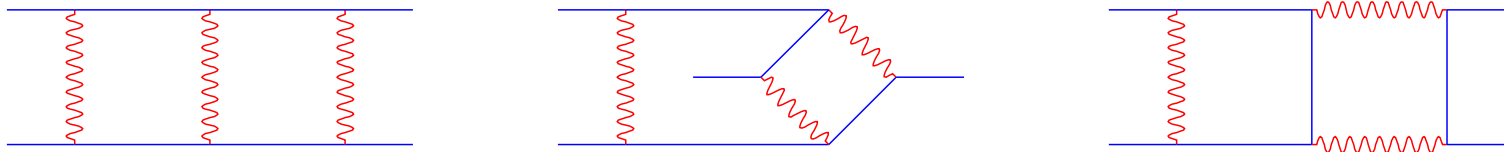
$$\begin{aligned} \mathcal{F} &= (-\mathbf{s}) \left\{ x_2 x_3 (x_4 + x_5 + x_6 + x_7) \right. \\ &\quad + x_5 x_6 (x_1 + x_2 + x_3 + x_4) \\ &\quad \left. + x_2 x_4 x_6 + x_3 x_4 x_5 \right\} \\ &\quad + (-\mathbf{t}) x_1 x_4 x_7 \end{aligned}$$

some examples (\* : no analytical result exists)

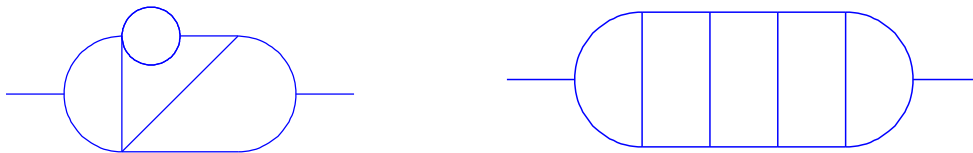
- \* massless 2-loop 4-point functions with 2 off-shell legs  
(planar and non-planar topologies)



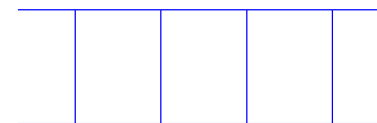
- (\* ) all 4-point master integrals needed for the calculation of 2-loop Bhabha scattering (massive fermions)



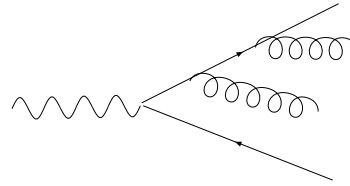
- (\* ) two-point-functions with 3, 4 and 5 loops, among them a 4-loop graph with an UV subdivergence, terms up to order  $\epsilon$  for 3-loop and 4-loop graphs



- the planar massless 3-loop 4-point-function with on-shell legs  
[V.A.Smirnov, May 03]



## Phase space integrals



integration over scaled invariants

$$x_1 = s_{12}/q^2, x_2 = s_{13}/q^2, x_3 = s_{23}/q^2, x_4 = s_{14}/q^2, x_5 = s_{24}/q^2, x_6 = s_{34}/q^2$$

example 1  $\rightarrow$  4 phase space:

$$\int d\Phi^{(4)} |M_4|^2 = C_{\Gamma}^{(4)} \int \prod_{j=1}^6 dx_j \delta(1 - \sum_{i=1}^6 x_i) [\lambda(x_1 x_6, x_2 x_5, x_3 x_4)]^{\frac{D-5}{2}} |M_4|^2$$

$$|M_4|^2 \sim \frac{\mathcal{P}_1(x_i, \epsilon)}{x_2^2 (x_2 + x_4 + x_6)^2} + \frac{\mathcal{P}_2(x_i, \epsilon)}{(x_2 + x_4 + x_6)(x_3 + x_5 + x_6)x_4 x_5} + \dots$$

$$\lambda(x, y, z) = 2(xy + xz + yz) - (x^2 + y^2 + z^2)$$

$\lambda \sim$  Gram determinant  $\Delta_4 = \det(G)$ ,  $G_{ij} = 2p_i \cdot p_j \rightarrow$  nonlinear constraint

application: master integrals for  $e^+e^- \rightarrow 2$  jets:

[A. Gehrmann-De Ridder, T. Gehrmann, G.H.]

$$\begin{aligned}
 R_4 &= \text{[Diagram: Circle with horizontal lines]} = \int d\Phi^{(4)} = P_4 \\
 R_6 &= \text{[Diagram: Circle with diagonal line]} = \int d\Phi^{(4)} \frac{1}{s_{134}s_{234}} \\
 R_{8,a} &= \text{[Diagram: Circle with two diagonal lines]} = \int d\Phi^{(4)} \frac{1}{s_{13}s_{23}s_{14}s_{24}} \\
 R_{8,b} &= \text{[Diagram: Circle with two diagonal lines]} = \int d\Phi^{(4)} \frac{1}{s_{13}s_{134}s_{23}s_{234}}
 \end{aligned}$$

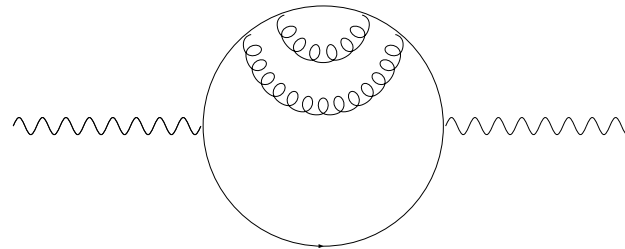
$$\begin{aligned}
 R_4 &= S_\Gamma(q^2)^{2-2\epsilon} [0.08335 + 0.8195\epsilon + 4.141\epsilon^2 + 14.40\epsilon^3 + 38.88\epsilon^4 + \mathcal{O}(\epsilon^5)] \\
 R_6 &= S_\Gamma(q^2)^{-2\epsilon} [0.64498 + 7.0423\epsilon + 40.507\epsilon^2 + \mathcal{O}(\epsilon^3)] \\
 R_{8,a} &= S_\Gamma(q^2)^{-2-2\epsilon} \left[ \frac{5.0003}{\epsilon^4} - \frac{0.0013}{\epsilon^3} - \frac{65.832}{\epsilon^2} - \frac{151.53}{\epsilon} + 37.552 + \mathcal{O}(\epsilon) \right] \\
 R_{8,b} &= S_\Gamma(q^2)^{-2-2\epsilon} \left[ \frac{0.74986}{\epsilon^4} - \frac{0.00009}{\epsilon^3} - \frac{14.001}{\epsilon^2} - \frac{52.911}{\epsilon} - 99.031 + \mathcal{O}(\epsilon) \right]
 \end{aligned}$$

agreement of numerical and analytical results better than 1%

without reduction to master integrals: [T.Binoth, G.H., hep-ph/0402265]

split into topologies ( $T_1 \dots T_8$ )

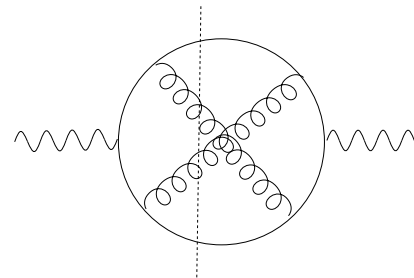
simple topology:



takes  $\sim 1$  hour for precision of 0.1% (Pentium IV 2.2 GHz)

most complicated topology:

$\sim 9$  hours for precision of 0.1%



1 → 5 phase space: 9 independent invariants

$$\int d\Phi^{(5)} = C_{\Gamma}^{(5)} \int \prod_{j=1}^{10} dx_j \delta(1 - \sum_{i=1}^{10} x_i) [-\Delta_5(\vec{x})]^{\frac{D-6}{2}} \Theta(-\Delta_5)$$

simplest example: 5-particle phase space volume

analytically: [A. Gehrmann-De Ridder, T. Gehrmann, G.H.]

$$\begin{aligned} \int d\Phi^{(5)} &= (4\pi)^{4\epsilon-7} \frac{\Gamma(1-\epsilon)^5}{2\Gamma(4-4\epsilon)\Gamma(5-5\epsilon)} \\ &= \frac{(4\pi)^{4\epsilon-7}}{\Gamma(1-2\epsilon)\Gamma(2-2\epsilon)} \left[ 0.0034722 + 0.0546875\epsilon \right. \\ &\quad \left. + 0.443355\epsilon^2 + 2.47433\epsilon^3 + 10.7292\epsilon^4 + \mathcal{O}(\epsilon^5) \right] \end{aligned}$$

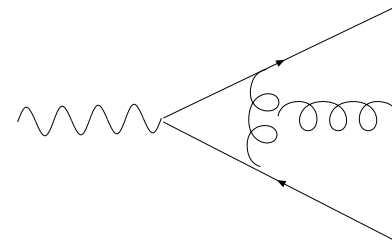
sector decomposition:

$$\begin{aligned} \int d\Phi^{(5)} &= \frac{(4\pi)^{4\epsilon-7}}{\Gamma(1-2\epsilon)\Gamma(2-2\epsilon)} \left[ 0.00347 + 0.05469\epsilon \right. \\ &\quad \left. + 0.44336\epsilon^2 + 2.47424\epsilon^3 + 10.7283\epsilon^4 + \mathcal{O}(\epsilon^5) \right] \end{aligned}$$

accuracy 0.5%, CPU time 10 minutes



## One loop + single unresolved combined:



- most complicated one-loop structure occurring in  $e^+e^- \rightarrow 2$  jets:  
box graph with one off-shell leg
- can be expressed by Hypergeometric functions  ${}_2F_1(1, -\epsilon, 1 - \epsilon; x_i/x_j)$   
( $x_1 = s_{12}/q^2, x_2 = s_{13}/q^2, x_3 = s_{23}/q^2$ )
- use parameter representation of  ${}_2F_1$

$${}_2F_1(1, -\epsilon, 1 - \epsilon; z) = \frac{\Gamma(1 - \epsilon)}{\Gamma(-\epsilon)} \int_0^1 dt t^{-1-\epsilon} (1 - tz)^{-1}$$

- combine with 3-particle phase space

$$\int d\phi_3 = \int dx_1 dx_2 dx_3 \delta(1 - x_1 - x_2 - x_3) (x_1 x_2 x_3)^{-\epsilon}$$

→ 4-dimensional parameter integral → sector decomposition

$e^+e^- \rightarrow 3$  jets: pentagons with one off-shell leg

$$\begin{aligned} I &= -\Gamma(3 + \epsilon) \int dz_i \delta(1 - \sum_{i=1}^5 z_i) \mathcal{F}^{3+\epsilon} \\ -\mathcal{F} &= s_{12} z_1 z_5 + s_{23} z_1 (z_3 + z_4 + z_5) + s_{13} z_1 (z_1 + z_2) \\ &\quad + s_{14} z_5 (z_1 + z_2 + z_3) + s_{24} z_1 (z_4 + z_5) + s_{34} (z_1 + z_2) (z_4 + z_5) \end{aligned}$$

sector decomposition  $\Rightarrow$

$$I = \sum_{\alpha=0}^2 P_\alpha / \epsilon^\alpha = \sum_{\alpha=0}^2 1 / \epsilon^\alpha \int_0^1 \prod_{i=1}^{4-\alpha} dt_i \mathcal{G}(t_i, s_{12}, \dots, s_{34}), \quad \lim_{t_i \rightarrow 0} \mathcal{G} \neq 0$$

insert into 4-particle phase space

$\Rightarrow$  proceed with decomposition in  $s_{12}, \dots, s_{34} \sim x_1, \dots, x_6$

# Structure of the program

**Input:** number  $N$  of propagators resp. invariants, integrand



loop/phase space subroutine



SECDEC → poles manifestly factorized



subtractions



Laurent series in  $\epsilon$



Creation of FORTRAN files



Numerical integration of finite functions (BASES, S. Kawabata)

## Subtractions:

$$\begin{aligned} & \int_0^1 dx x^{-1+\kappa\epsilon} \mathcal{F}(x, y) \\ &= \frac{1}{\kappa\epsilon} \int_0^1 dx \mathcal{F}(x, y) \delta(x) + \int_0^1 dx x^{-1+\kappa\epsilon} [\mathcal{F}(x, y) - \mathcal{F}(0, y)] \\ &= \frac{1}{\kappa\epsilon} \int_0^1 dx \mathcal{F}(x, y) \delta(x) + \sum_{n=0}^{\infty} \frac{(\kappa\epsilon)^n}{n!} \int_0^1 dx \left[ \frac{\ln^n(x)}{x} \right]_+ \mathcal{F}(x, y) \end{aligned}$$

→ same procedure for all  $x_i$

→ Laurent series

$$\mathcal{I} = \sum_{k=-a}^b \epsilon^k C_k + \mathcal{O}(\epsilon^{b+1})$$

→ inclusion of measurement function straightforward!

# Summary and outlook

- Automated sector decomposition algorithm: powerful method to isolate overlapping infrared poles and to calculate numerically
  - multi-loop integrals
  - one-loop + real emission combined
  - double real radiation at NNLO
- advantages of the method:
  - robust and multi-purpose
  - double real emission:
    - no need to establish a subtraction scheme and to integrate analytically over complicated subtraction terms
    - inclusion of measurement function no problem  $\rightarrow$  differential
    - generalisation to other processes than  $e^+e^-$  annihilation feasible
- drawbacks:
  - loop integrals with more than one scale: only Euclidean points so far
  - generates large number of (finite) functions