# A numerical approach to the double real radiation part of $e^{+} e^{-} \rightarrow 3$ jets at NNLO 

Gudrun Heinrich

Universität Zürich


## Motivation

experiments at high energy colliders in past years:

## precision measurements

led to stringent tests of the Standard Model and bounds on New Physics only possible in combination with

## "precision calculations"

what to expect from "Old Physics" must be well under control $\Rightarrow$ precise knowledge of parameters like $\alpha_{s}, \sin ^{2} \theta_{W}$ important

- at the LHC : $n$-jet cross section $\sim \alpha_{s}^{n}$
- future International Linear Collider will reach precision at the per mille level


## Jet production in $e^{+} e^{-}$annihilation

measurements of $e^{+} e^{-} \rightarrow$ jet rates \& shape observables

- allow precision tests of the SM over wide range of energies
- offer possibility for determination of strong coupling constant $\alpha_{s}$ with unseen precision
$\alpha_{s}$ world average:
$\alpha_{s}\left(M_{Z}\right)=0.1182 \pm 0.0027$ (stat. and sys.) [s. Bethke 04]
determination based only on data where
NNLO QCD theory predictions exist !
(DIS, $\Gamma(Z \rightarrow$ had), $\tau, \Upsilon-$ decays)


## $\alpha_{s}$ determination

LEP data for jets and shape observables very precise, but not used for world average : only NLO theory available!


## $\alpha_{s}$ determination

error on $\alpha_{s}\left(M_{Z}\right)$ from $e^{+} e^{-}$jet rates and event shape observables (NLO + NLL resum) :
theoretical: $\mathcal{O}(5 \%)$, dominated by scale dependence! experimental: $\mathcal{O}(1.3 \%)$ (statistical, hadronisation, ...)
[R. Jones, Ford, Salam, Stenzel, Wicke '04]
$\Rightarrow$ NNLO will improve the error considerably ! mandatory to match experimental precision at the ILC

NLO calculation:
Ellis, Ross, Terrano '81, Fabricius, Schmitt, Kramer, Schierholz '81,
Kramer, Lampe '89, Kunszt, Nason, Marchesini, Webber '89
resummation:
Catani et al. '92-'98, Dokshitzer et al. '98, Banfi et al. '02, Gardi et al. '01-'03

## NNLO calculations

problems in NNLO calculations:

- enormous complexity of expressions
- analytic integrations very difficult
- direct numerical evaluation hampered by singularities
- massless particles $\Rightarrow$ soft and collinear (IR) singularities ( $1 / \epsilon^{n}$ poles in dim.reg.)
- IR singularities are entangled in a complicated way
$\Rightarrow$ need to be isolated and subtracted
- from loop integrals ( $\rightarrow$ analytic integration)
- from integrals over soft/collinear phase space regions ( $\rightarrow$ subtraction terms)


## subtraction of infrared poles: NLO

virtual: $d \sigma^{V}=P_{2} / \epsilon^{2}+P_{1} / \epsilon+P_{0}$
real: integration of subtraction terms $d \sigma^{S}$ over singular regions of phase space

$$
\Rightarrow \int_{\text {sing }} d \sigma^{S}=-P_{2} / \epsilon^{2}-P_{1} / \epsilon+Q_{0}
$$



## partonic ingredients for $e^{+} e^{-} \rightarrow 3$ jets at NNLO

-2-loop virtual

- one-loop plus single unresolved real emission

- double unresolved real emission
bottleneck: 5 partons in final state, up to 2 soft or collinear


## difficulty: isolation of infrared poles

 from phase space integrals
## subtraction of infrared poles: NNLO

$m$-jet production schematically:

$$
\begin{aligned}
& \mathrm{d} \sigma_{N N L O}= \underbrace{\int_{\mathrm{d} \Phi_{m+2}}\left(\mathrm{~d} \sigma_{N N L O}^{R}-\mathrm{d} \sigma_{N N L O}^{S}\right)}_{\text {finite }}+\int_{\mathrm{d} \Phi_{m+2}} \mathrm{~d} \sigma_{N N L O}^{S} \\
&+\underbrace{\int_{\mathrm{d} \Phi_{m+1}}\left(\mathrm{~d} \sigma_{N N L O}^{V, 1}-\mathrm{d} \sigma_{N N L O}^{V S, 1}\right)}_{\text {finite }}+\int_{\mathrm{d} \Phi_{m+1}} \mathrm{~d} \sigma_{N N L O}^{V S, 1} \\
&+\int_{\mathrm{d} \Phi_{m}} \mathrm{~d} \sigma_{N N L O}^{V, 2} \\
& \int_{\mathrm{d} \Phi_{m+2}} \mathrm{~d} \sigma_{N N L O}^{S}+\int_{\mathrm{d} \Phi_{m+1}} \mathrm{~d} \sigma_{N N L O}^{V S, 1}+\int_{\mathrm{d} \Phi_{m}} \mathrm{~d} \sigma_{N N L O}^{V, 2}=\text { finite }
\end{aligned}
$$

## subtraction of infrared poles: NNLO

two conceptually different approaches:

- "conventional" approach:
manual construction of a subtraction scheme and analytic integration over subtraction terms in
$D=4-2 \epsilon$ dimensions
[A. Gehrmann-De Ridder, T. Gehrmann, N. Glover], [Kilgore], [Weinzierl],
[Del Duca, Somogyi, Trocsanyi], [Frixione, Grazzini]
- sector decomposition: automated isolation of IR poles in parameter space and numerical integration of pole coefficients
[Binoth, GH], [Anastasiou, Melnikov, Petriello]


## sector decomposition

- no manual construction of subtraction terms
- isolation of poles in $1 / \epsilon$ by automated procedure acting in parameter space
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- application to real radiation [GH L\&L '02; Anastasiou, Melnikov, Petriello, Binoth, GH '03/04]
- development as a powerful tool for differential NNLO calculations [Anastasiou, Melnikov, Petriello: $e^{+} e^{-} \rightarrow 2$ jets, $H$ production, $\mu$ decay, $W$ production '04-06]


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- $e^{+} e^{-} \rightarrow 3$ jets at NNLO: very complicated singularity structure due to high number of massless particles


## basics of sector decomposition

integral of matrix element squared with some measurement function $\mathcal{J}$ :
typically contains "overlapping" structures like

$$
\begin{aligned}
\int \mathrm{d} \Phi^{(D)}|\mathrm{ME}|^{2} \mathcal{J} & \sim \int \mathrm{~d} s_{13} \mathrm{~d} s_{23} s_{13}^{-1-\epsilon} \frac{\mathcal{J}\left(s_{13}, s_{23}\right)}{s_{13}+s_{23}} \\
& \sim \int_{0}^{1} d x d y x^{-1-\epsilon} \frac{\mathcal{J}(x, y)}{x+y}
\end{aligned}
$$

singularities for $x, y \rightarrow 0$ need to be factorised
sector decomposition is an algorithmic way to factorise this type of entangled singularities

## sector decomposition

$$
I=\int_{0}^{1} d x d y x^{-1-\epsilon}(x+y)^{-1} \mathcal{J}(x, y)[\underbrace{\Theta(x-y)}_{(1)}+\underbrace{\Theta(y-x)}_{(2)}]
$$

$$
\text { subst. (1) } y=x t \quad(2) x=y t
$$

$$
\begin{aligned}
I= & \int_{0}^{1} d x x^{-1-\epsilon} \int_{0}^{1} d t(1+t)^{-1} \mathcal{J}(x, x t) \\
& +\int_{0}^{1} d y y^{-1-\epsilon} \int_{0}^{1} d t t^{-1-\epsilon}(1+t)^{-1} \mathcal{J}(y t, y)
\end{aligned}
$$

$\Rightarrow$ singularities factorised, number of integrals doubled

## general algorithm

- map parameter integrals to unit hypercube (manual)
- map singularities to be located at the origin of parameter space (manual/automated)


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## result:

$$
\begin{aligned}
I= & \int_{0}^{1} d x_{1} x_{1}^{b_{1}-\kappa_{1} \epsilon} \ldots \int_{0}^{1} d x_{n} x_{n}^{b_{n}-\kappa_{n} \epsilon} F\left(x_{1}, \ldots, x_{n}\right) \\
& \lim _{x_{i} \rightarrow 0} F\left(x_{1}, \ldots, x_{n}\right)=\mathrm{const}
\end{aligned}
$$

## general algorithm

- perform subtractions and expansion in $\epsilon$ (fully automated)
use identities like

$$
\begin{aligned}
& \int_{0}^{1} d x \int_{0}^{1} d y x^{-1-\kappa \epsilon} f(x, y)= \\
& -\frac{1}{\kappa \epsilon} \int_{0}^{1} d x \delta(x) \int_{0}^{1} d y f(x, y)+\int_{0}^{1} d x \int_{0}^{1} d y x^{-\kappa \epsilon} \frac{f(x, y)-f(0, y)}{x}
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note: if $f(x, y)=\Theta(x-a) g(y) \Rightarrow$ pole term zero

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\end{aligned}
$$

- result after $\epsilon$-expansion: Laurent series in $\epsilon$

$$
I=\sum_{k=\text { maxpole }}^{-n} C_{k}\left(y_{i}\right) / \epsilon^{k}+\mathcal{O}\left(\epsilon^{n+1}\right) \quad\left(y_{i} \text { scaled invariants } s_{i j}\right)
$$

- poles are isolated $\Rightarrow$ integrate finite coefficient functions $C_{k}\left(y_{i}\right)$ numerically over the phase space


## application to $1 \rightarrow 5$ parton phase space

use scaled invariants $y_{1}=s_{12} / q^{2}, \ldots, y_{10}=s_{45} / q^{2}$

$$
\int d \Phi_{1 \rightarrow 5}^{D}=C_{\Gamma}^{(5)} \int \prod_{j=1}^{10} d y_{j} \delta\left(1-\sum_{i=1}^{10} y_{i}\right)\left(-\Delta_{5}\right)^{\frac{D}{2}-3} \Theta\left(-\Delta_{5}\right)
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\Delta_{5}= & y_{10}^{2} y_{1} y_{2} y_{3}+y_{9}^{2} y_{1} y_{4} y_{5}+y_{8}^{2} y_{2} y_{4} y_{6}+y_{7}^{2} y_{3} y_{5} y_{6} \\
& +y_{6}^{2} y_{1} y_{7} y_{8}+y_{5}^{2} y_{2} y_{7} y_{9}+y_{4}^{2} y_{3} y_{8} y_{9}+y_{3}^{2} y_{4} y_{7} y_{10} \\
& +y_{2}^{2} y_{5} y_{8} y_{10}+y_{1}^{2} y_{6} y_{9} y_{10} \\
& +y_{10}\left[y_{2} y_{3} y_{5} y_{7}+y_{1} y_{3} y_{6} y_{7}+y_{2} y_{3} y_{4} y_{8}\right. \\
& \left.+y_{1} y_{2} y_{6} y_{8}+y_{1} y_{3} y_{4} y_{9}+y_{1} y_{2} y_{5} y_{9}\right] \\
& +y_{9}\left[y_{4} y_{5}\left(y_{3} y_{7}+y_{2} y_{8}\right)+y_{1} y_{6}\left(y_{5} y_{7}+y_{4} y_{8}\right)\right] \\
& +y_{6} y_{7} y_{8}\left(y_{3} y_{4}+y_{2} y_{5}\right)
\end{aligned}
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can be done once and for all, but costly in number of iterations for certain denominators better:


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- perform variable transformations to map integrations to unit hypercube (solve constraint $\Delta_{5}=0$ )
can be done once and for all, but costly in number of iterations for certain denominators better:
- use different parametrisations, optimized for certain denominator structures ("topologies")
(minimise square-root terms in denominators, maximize natural factorisations)


## example from $e^{+} e^{-} \rightarrow 3$ jets

## example:


convenient phase space parametrisation:
$s_{1345} / q^{2}=t_{1}, s_{134} / q^{2}=t_{1} t_{2}, s_{13} / q^{2}=t_{1} t_{2} t_{3}, \ldots$
$s_{24} / q^{2}=y_{5}^{-}+\left(y_{5}^{+}-y_{5}^{-}\right) t_{5}, y_{5}^{ \pm}$solution of $\Delta_{5}=0$,
$s_{25}, s_{45}$ also contain square-roots

$$
\begin{aligned}
\int d \Phi_{1 \rightarrow 5}^{D}= & \mathcal{K}_{\Gamma}^{(5)}\left(q^{2}\right)^{2 D-5} \int_{0}^{1} \prod_{j=1}^{9} d t_{j} t_{1}^{2-3 \epsilon}\left[t_{5}\left(1-t_{5}\right)\right]^{-1-\epsilon}\left[t_{8}\left(1-t_{8}\right) t_{9}\left(1-t_{9}\right)\right]^{-\frac{1}{2}-\epsilon} \\
& {\left[\left(1-t_{1}\right) t_{2}\left(1-t_{2}\right)\left(1-t_{3}\right)\right]^{1-2 \epsilon}\left[t_{3} t_{4}\left(1-t_{4}\right) t_{6}\left(1-t_{6}\right) t_{7}\left(1-t_{7}\right)\right]^{-\epsilon} }
\end{aligned}
$$

## example from $e^{+} e^{-} \rightarrow 3$ jets

## result for example graph $T_{5}$ :



$$
\begin{aligned}
T_{5}= & C_{F}^{3}\left(\frac{\alpha_{s}}{4 \pi}\right)^{3} T_{2}\left\{-\frac{0.166618 \pm 0.000086}{\epsilon^{3}}\right. \\
& -\frac{1}{\epsilon^{2}}\left[(1.49928 \pm 0.00148)-(0.499853 \pm 0.000258) \log \left(\frac{Q^{2}}{\mu^{2}}\right)\right] \\
& -\frac{1}{\epsilon}\left[(5.59588 \pm 0.0064)-(4.49783 \pm 0.0044) \log \left(\frac{Q^{2}}{\mu^{2}}\right)\right. \\
& \left.\left.+(0.749779 \pm 0.00039) \log ^{2}\left(\frac{Q^{2}}{\mu^{2}}\right)\right]+ \text { finite }\right\}
\end{aligned}
$$

## check by Kinoshita-Lee-Nauenberg theorem


renormalisation constants:
$z_{1}=C_{F} \frac{\alpha_{s}}{4 \pi} \frac{1}{\epsilon}, z_{2}=C_{F}^{2}\left(\frac{\alpha_{s}}{4 \pi}\right)^{2}\left(\frac{1}{2 \epsilon^{2}}-\frac{1}{4 \epsilon}\right), z_{3}=C_{F}^{3}\left(\frac{\alpha_{s}}{4 \pi}\right)^{3}\left(\frac{1}{6 \epsilon^{3}}-\frac{1}{4 \epsilon^{2}}+\frac{1}{6 \epsilon}\right)$
e.g. $z_{3}$ from


## check pole cancellations

$$
\begin{aligned}
& z_{1} T_{4}+z_{2} T_{3}+z_{3} T_{2}= \\
& C_{F}^{3}\left(\frac{\alpha_{s}}{4 \pi}\right)^{3} T_{2}\left\{\frac{1}{6 \epsilon^{3}}+\frac{1}{2 \epsilon^{2}}\left[3-\log \left(\frac{Q^{2}}{\mu^{2}}\right)\right]\right. \\
& \left.+\frac{1}{\epsilon}\left[5.60813-\frac{9}{2} \log \left(\frac{Q^{2}}{\mu^{2}}\right)+\frac{3}{4} \log ^{2}\left(\frac{Q^{2}}{\mu^{2}}\right)\right]+\text { finite }\right\} \\
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## differential results

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- in order to compare to experimental data, we need to produce distributions which are differential in certain observables
- no problem: before numerical integration, pole coefficients and finite parts are functions of invariants $s_{12}, \ldots, s_{45}$
$\Rightarrow$ 4-momenta of all final state particles can be reconstructed
$\Rightarrow$ program has architecture of partonic event generator
$\Rightarrow$ flexibility to include experimental cuts, jet algorithms, definition of shape observables, etc. at the Monte Carlo level


## example

## 3,4,5-jet rates for "ladder" contribution



- virtual contributions calculated analytically
(only renormalisation factors for ladder graph)
- phase space integrations for 3,4,5-parton final states by Monte Carlo program based on output of sector decomposition for $T_{4}$ and $T_{5}$


## example: jet rates for ladder graph


$y^{\text {cut }}$ : miminal separation between jets
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## note:


$y^{\text {cut }}$ : miminal separation between jets
in terms of invariant mass (JADE jet algorithm)

- ladder graph only, not a physical observable, but architecture of program as a partonic event generator same for remaining parts
- CPU time $\mathcal{O}(10 \mathrm{~min})$ for $1 \%$ precision (2.8 GHz Pentium IV)


## a non-planar topology

more complex because square-root term in denominator unavoidable



## a non-planar topology

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note:

- virtual corrections not yet included
- CPU time $\mathcal{O}(2 \mathrm{~h})$ for $1 \%$ precision
- other topologies can be calculated in parallel
- $\mathcal{O}(100)$ topologies

- $\mathcal{O}(10)$ PS parametrisations


## roadmap

- include all topologies of $e^{+} e^{-} \rightarrow q \bar{q} g g g, q \bar{q} Q \bar{Q} g$ squared matrix elements
limit size of expressions produced by iterated sector decomposition by using convenient phase space parametrisations and information on physical limits
- combine with one-loop + single real and two-loop virtual corrections
- one-loop + single real: use a combination of analytic integration and sector decomposition
- two-loop virtual: use analytic expressions to save CPU time
[Garland, Gehrmann, Glover, Koukoutsakis, Remiddi '01],
[Moch, Uwer, Weinzierl '02]


## Summary: comparison of the two approaches

## analytic subtraction

moderate number of subtraction termsmaximal (analytical) control over pole parts
insights into infrared structure of QCD
different for each colour structure
analytical integration of subtraction terms may become impossible for processes involving several mass scales

## sector decomposition

produces large expressions
numerical cancellation of pole coefficients
$\oplus$ high level of automatisation
basic algorithm same for all colour structures of a given process
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the two methods are complementary

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the sector decomposition approach has been/will be a useful tool for NNLO calculations where analytical methods reach their limits

## backup

for Monte Carlo program: remap to energies and angles

$$
\begin{aligned}
& E_{1}=\frac{q^{2}-s_{2345}}{2 q}, E_{2}=\frac{q^{2}-s_{1345}}{2 q}, \\
& E_{3}=\frac{q^{2}-s_{1245}}{2 q}, E_{4}=\frac{q^{2}-s_{1235}}{2 q}
\end{aligned}
$$

$$
\cos \theta_{1}=-1+2\left(s_{1345} s_{2345}-s_{345}\right) /\left(1-s_{1345}\right) /\left(1-s_{2345}\right)
$$

$$
\cos \theta_{2}=-1+2\left(s_{1245} s_{2345}-s_{245}\right) /\left(1-s_{1245}\right) /\left(1-s_{2345}\right)
$$

$$
\cos \theta_{3}=-1+2\left(s_{1235} s_{2345}-s_{235}\right) /\left(1-s_{1235}\right) /\left(1-s_{2345}\right)
$$

