## **Higher orders with Monte Carlo methods**

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in collaboration with

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I: Multileg NLO calculations

II: Local subtraction terms

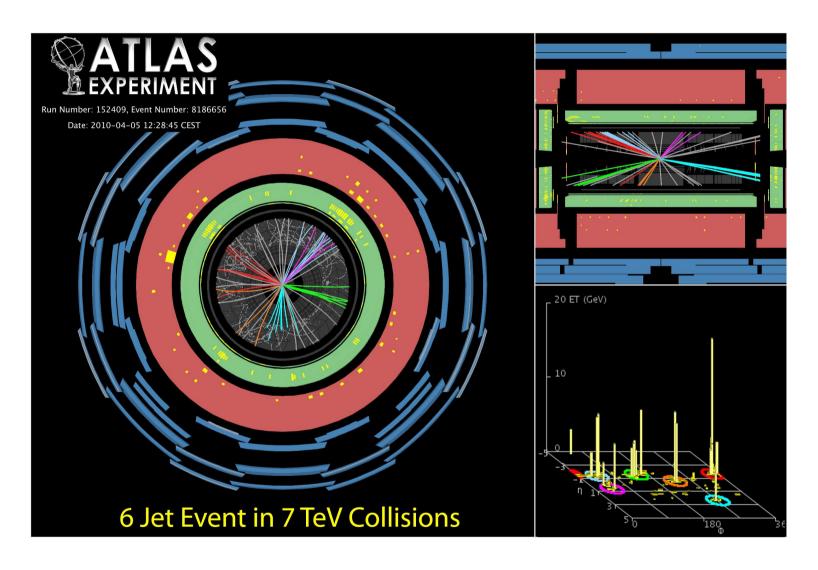
**III:** Contour deformation

IV: Efficiency

V: Results

**VI**: Extension to higher orders

## **LHC** physics



Jets: A bunch of particles moving in the same direction

## **Multileg NLO calculations**

#### What one aims for:

- NLO calculations for multi-parton processes at the LHC. Multi-parton processes: 3, 4, 5, 6, ... partons in the final state.
- For a given process the program should be usable for any infrared-safe observable.
- Need to compute the virtual corrections and the real corrections.

### Conventional set-up for NLO calculations

Need Born, real contribution and virtual contribution:

- Efficient methods known for Born and real contribution.
- Subtraction method or phase-space slicing is used to render the real contribution finite.
- Loop integrals in the virtual contribution are reduced (numerically) to a few master integrals.
- Integration over the loop momentum in the master integrals is done analytically.
- Integration over momenta of the final state particles is done by Monte Carlo.

### Conventional set-up for the virtual part

Based on Feynman diagrams: avoid instabilities due to Gram determinants

Based on unitarity and cut techniques: avoid instabilities in solving linear systems of equations

#### Recent results:

- $pp \rightarrow W/Z + 4$  jets,
- $pp \rightarrow WW + 2$  jets,
- $pp \rightarrow t\bar{t} + 2$  jets,
- $e^+e^- \rightarrow 5$  jets,

Berger et al. (Blackhat collaboration), Ellis, Melnikov, Zanderighi, Melia, Rontsch, Bevilacqua, Czakon, Pittau, Papadopoulos, Worek, Bredenstein, Denner, Dittmaier, Pozzorini, Hirschi, Frederix, Frixione, Garzelli, Maltoni, ...

### The subtraction method for the real emission

The subtraction methods subtracts out a simple term, which approximates the real emission in all singular limits:

$$\int_{n+1} d\sigma^{R} + \int_{n} d\sigma^{V} = \int_{\underbrace{n+1}} \left( d\sigma^{R} - d\sigma^{A} \right) + \int_{\underbrace{n} \text{ singular}} \mathbf{I} \otimes d\sigma^{B} + \int_{n} d\sigma^{V}$$

- Residue subtraction: Frixione, Kunszt and Signer, '95; Del Duca, Somogyi, Trócsányi, '05
- Dipole subtraction: Catani and Seymour '96; Phaf and S.W. '01; Catani, Dittmaier, Seymour and Trócsányi '02;
   Nagy and Soper, '07; Dittmaier and Kasprzik, '08; Czakon, Papadopoulos and Worek, '09; Chung, Kramer and Robens, '10
- Antenna subtraction: Kosower, '97; Gehrmann-De Ridder, Gehrmann, Glover, '05

### **Computational costs**

- Efficient methods like recursion relations known for Born and real contribution.
- Integration over momenta of the final state particles is done by Monte Carlo.
- Real emission (minus the subtraction terms) can be automated.
   S.W., '05, T. Gleisberg and F. Krauss, '07, M. Seymour and C. Tevlin, '08, K. Hasegawa, S. Moch and P. Uwer, '08, R. Frederix, T. Gehrmann and N. Greiner, '08, M. Czakon, C. Papadopoulos and M. Worek, '09.
- Insertion term  $\mathbf{I} \otimes d\sigma^B$  is cheap.
- Virtual corrections usually reduced to a set of master integrals, which are known analytically.
  - Evaluation time usually less or equal to real part.
- CPU-time for real emission sets time scale.

### Our approach: Never change a winning team

### Do the loop integrals numerically with Monte Carlo techniques!

- Can combine phase space integration (3n-4 dimensions) with loop integration (4 dimensions) in one Monte Carlo integration.
- Monte Carlo integration error scales with  $1/\sqrt{N}$ , independent of the dimension.

But: Loop integrals are divergent and need regularization. They are therefore calculated in  $D=4-2\epsilon$  dimensions

$$\int d^{4-2\varepsilon}k \ f(k) = \frac{c_2}{\varepsilon^2} + \frac{c_1}{\varepsilon} + c_0 + O(\varepsilon)$$

Idea: Subtraction method.

$$\int d^{4-2\varepsilon}k \ f(k) = \underbrace{\int d^{4-2\varepsilon}k \ [f(k) - g(k)]}_{\text{convergent}} + \underbrace{\int d^{4-2\varepsilon}k \ g(k)}_{\text{simple}}$$

### Subtraction method for loop integrals

Use subtraction also for the virtual part:

$$\int_{n+1} d\sigma^{R} + \int_{n} d\sigma^{V} = \int_{n+1} \left( d\sigma^{R} - d\sigma^{A} \right) + \int_{n} \left( \mathbf{I} + \mathbf{L} \right) \otimes d\sigma^{B} + \int_{n} \left( d\sigma^{V} - d\sigma^{A'} \right)$$
convergent finite convergent

- In the last term  $d\sigma^V d\sigma^{A'}$  the Monte Carlo integration is over a phase space integral of n final state particles plus a 4-dimensional loop integral.
- ullet All explicit poles cancel in the combination  ${f I}+{f L}.$
- Divergences of one-loop amplitudes related to IR-divergences (soft and collinear) and to UV-divergences.

### **Numerical NLO QCD calculations**

Proceed through the following steps:

- 1. Local subtraction terms for soft, collinear and ultraviolet singular part of the integrand of one-loop amplitudes
- 2. Contour deformation for the 4-dimensional loop integral.
- 3. Numerical Monte Carlo integration over phase space and loop momentum.

Not a new idea: Nagy and Soper proposed in '03 this method, working graph by graph.

(see also: Soper; Krämer, Soper; Catani et al.; Kilian, Kleinschmidt)

What is new: The IR-subtraction terms can be formulated at the level of amplitudes,

no need to work graph by graph.

The IR-subtraction terms are universal and amasingly simple.

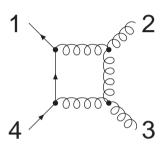
### **Primitive amplitudes**

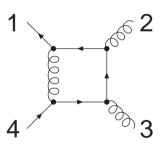
Colour-decomposition of one-loop amplitudes:

$$\mathcal{A}^{(1)} = \sum_j C_j A_j^{(1)}.$$

Primitive amplitudes distinguished by:

- fixed cyclic ordering
- definite routing of the fermion lines
- particle content circulating in the loop



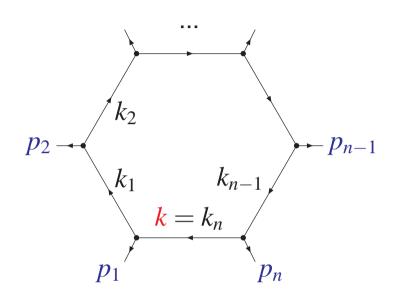


### **Notation and kinematics**

All momenta specified by  $p_1, ..., p_n$  and k:

$$k_i = k - (p_1 + \dots + p_i)$$

For cyclic ordered amplitudes we have only n different propagators.



Write primitive one-loop amplitude as

$$A_{\mathrm{bare}}^{(1)} = \int \frac{d^D k}{(2\pi)^D} G_{\mathrm{bare}}^{(1)}, \qquad G_{\mathrm{bare}}^{(1)} = P(k) \prod_{i=1}^n \frac{1}{k_i^2 - m_i^2 + i\delta}.$$

P(k) is a polynomial in k.

Integrand can be calculated efficiently using recursion relations.

### The infrared subtraction terms for the virtual corrections

### Local unintegrated form:

$$G_{\text{soft+coll}}^{(1)} = -4\pi\alpha_s i \sum_{i \in I_g} \left( \frac{4p_i p_{i+1}}{k_{i-1}^2 k_i^2 k_{i+1}^2} - 2 \frac{S_i g_{i-1,i}^{UV}}{k_{i-1}^2 k_i^2} - 2 \frac{S_{i+1} g_{i,i+1}^{UV}}{k_i^2 k_{i+1}^2} \right) A_i^{(0)}.$$

with  $S_q = 1$ ,  $S_g = 1/2$ . The function  $g_{i,j}^{UV}$  provides damping in the UV-region:

$$\lim_{k\to\infty}g_{i,j}^{UV}=\mathcal{O}\left(k^{-2}\right),\qquad \lim_{k_i\mid\mid k_j}g_{i,j}^{UV}=1.$$

### Integrated form:

$$S_{\varepsilon}^{-1}\mu^{2\varepsilon} \int \frac{d^{D}k}{(2\pi)^{D}} G_{\text{soft+coll}}^{(1)} = \frac{\alpha_{s}}{4\pi} \frac{e^{\varepsilon \gamma_{E}}}{\Gamma(1-\varepsilon)} \sum_{i \in I_{g}} \left[ \frac{2}{\varepsilon^{2}} \left( \frac{-2p_{i} \cdot p_{i+1}}{\mu^{2}} \right)^{-\varepsilon} + \frac{2}{\varepsilon} (S_{i} + S_{i+1}) \left( \frac{\mu_{\text{UV}}^{2}}{\mu^{2}} \right)^{-\varepsilon} \right] A_{i}^{(0)} + \mathcal{O}(\varepsilon),$$

M. Assadsolimani, S. Becker, S.W., '09

### **UV-subtraction terms**

In a fixed direction in loop momentum space the amplitude has up to quadratic UV-divergences.

Only the integration over the angles reduces this to a logarithmic divergence.

For a local subtraction term we have to match the quadratic, linear and logarithmic divergence.

The subtraction terms have the form of counter-terms for propagators and vertices.

The complete UV-subtraction term can be calculated recursively.

S. Becker, Ch. Reuschle, S.W., JHEP 1012 (2010), 013, arxiv:1010.4187

### **UV-subtraction terms**

Example: The quark-gluon vertex.

### Local unintegrated form:

$$= ig^{3}S_{\varepsilon}^{-1}\mu^{4-D}\int \frac{d^{D}k}{(2\pi)^{D}i} \frac{2(1-\varepsilon)\bar{k}/\gamma^{\mu}\bar{k}/+4\mu_{UV}^{2}\gamma^{\mu}}{(\bar{k}^{2}-\mu_{UV}^{2})^{3}}$$

### Integrated form:

$$= i \frac{g^3}{(4\pi)^3} \gamma^{\mu} (-1) \left( \frac{1}{\epsilon} - \ln \frac{\mu_{UV}^2}{\mu^2} \right) + \mathcal{O}(\epsilon)$$

We can ensure that the integrated expression is proportional to the Born.

### **Contour deformation**

With the subtraction terms for UV- and IR-singularities one removes

- UV divergences
- Pinch singularities due to soft or collinear partons

#### Still remains:

- Singularities in the integrand, where a deformation into the complex plane of the contour is possible.
- Pinch singularities for exceptional configurations of the external momenta (thresholds, anomalous thresholds ...), integrable over phase space and loop space.

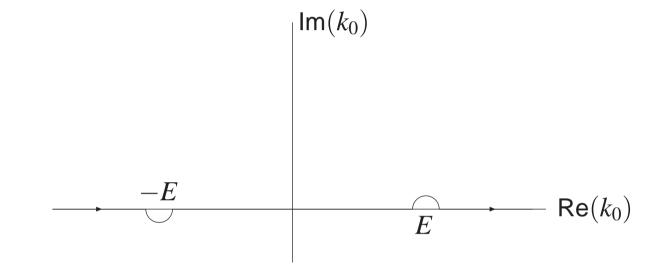
### **Contour deformation**

$$I = \int d^4k \, \underbrace{[f(k) - g(k)]}_{h(k)}$$

h(k) meromorphic function of four complex variables  $k_0, k_1, k_2, k_3$ .

Integration over a surface of (real) dimension 4 in  $\mathbb{C}^4$ .

*I* independent of the choice of the surface, as long as no poles are crossed.



What is the best choice for the surface, in order to minimize Monte Carlo integration errors?

### **Contour deformation**

We work with two methods for the contour deformation:

Direct deformation, entirely in the space of the loop momentum.
 Integration is over the loop momentum k.
 At present only for massless particles.

Gong, Nagy, Soper, '09; Becker, Reuschle, S.W., '12

Additional Feynman parameters.

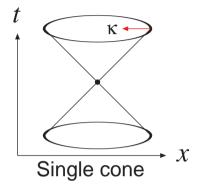
Integration is over the loop momentum k and the Feynman parameters  $\alpha$ . General, but slightly less efficient.

Nagy, Soper, '06; Anastasiou, Beerli, Daleo, '07; Becker, Reuschle, S.W., '10

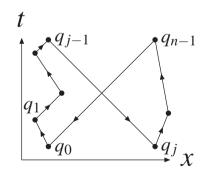
### **Direct contour deformation**

Deformation of the loop momentum:

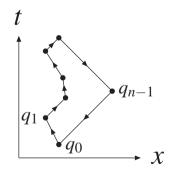
$$k_{\mathbb{C}} = k_{\mathbb{R}} + i\kappa$$



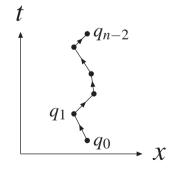
For n cones draw only the origins of the cones:



generic with 2 initial partons



initial partons adjacent



no initial partons

### **Efficiency**

With the local subtraction terms and the contour deformation we obtain an integral, where the loop integration can – in principle – be performed with Monte Carlo methods.

However, the integrand is oscillating:

$$I = \int_{0}^{1} dx \left[ c + \mathbf{A} \sin(2\pi x) \right], \quad \mathbf{A} \gg \mathbf{c}$$

This leads to large Monte Carlo integration errors.

Solution: Antithetic variates: Evaluate the integrand at x and (1-x).

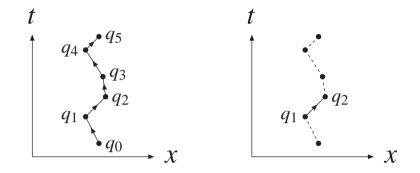
### Infrared channels

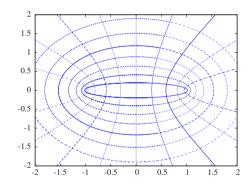
### Non-holomorphic splitting:

$$I_{\text{int}} = \sum_{i} \int \frac{d^4k}{(2\pi)^4} w_i(k) f(k),$$

### Weights:

$$w_i(k) = \frac{\left(\frac{1}{|k_i^2||k_{i+1}^2|}\right)^{\alpha}}{\sum_{j} \left(\frac{1}{|k_j^2||k_{j+1}^2|}\right)^{\alpha}},$$



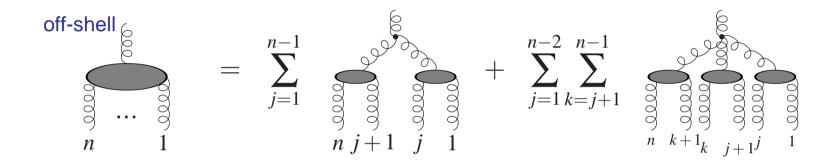


Coordinate system, where a line segment  $[q_i, q_{i+1}]$  is singled out: Generalised elliptical coordinates

Use technique of antithetic variates in these coordinates.

### **Recurrence relations**

Off-shell currents provide an efficient way to calculate amplitudes:



No Feynman diagrams are calculated in this approach!

F. A. Berends and W. T. Giele

## The one-loop recurrence relations

$$= \sum_{i=m}^{n+1} \sum_{i=m}^{n+$$

$$+\sum_{i=m}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n+1}\sum_{i=m}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=i+$$

$$+\sum_{i=m}^{n-1}\sum_{\substack{n+1\\00000}}^{m}\sum_{\substack{i=n\\i=m}}^{n-1}\sum_{\substack{n+1\\00000}}^{m}\sum_{\substack{i=n\\i=m}}^{n-1}\sum_{\substack{n+1\\00000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\00000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\00000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\00000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\0000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{n+1\\0000000}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{i=n}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{i=n}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum_{\substack{i=n\\i=m}}^{m}\sum$$

### The recurrence relation for the UV-counterterm

$$=\sum_{i=m}^{n+1} \left[ \sum_{i=m}^{n+1} \left( \sum_{i=1}^{n+1} \sum_{i=m}^{n+1} \left( \sum_{i=1}^{n+1} \sum_{i=m}^{n+1} \sum_{i=m}^{n+1} \sum_{i=m}^{n+1} \sum_{i=m}^{n+1} \sum_{i=m}^{n+1} \sum_{i=1}^{n+1} \sum_{i$$

$$+\sum_{i=m}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=$$

$$+\sum_{i=m}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n+1}\sum_{j=i+1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{j=i+1}^{n+1}\sum_{j=$$

### Results

We test our approach by calculating the NLO corrections for n-jet production in electron-positron annihilation in the leading colour approximation.

Results for n = 2, 3, 4 are well-known.

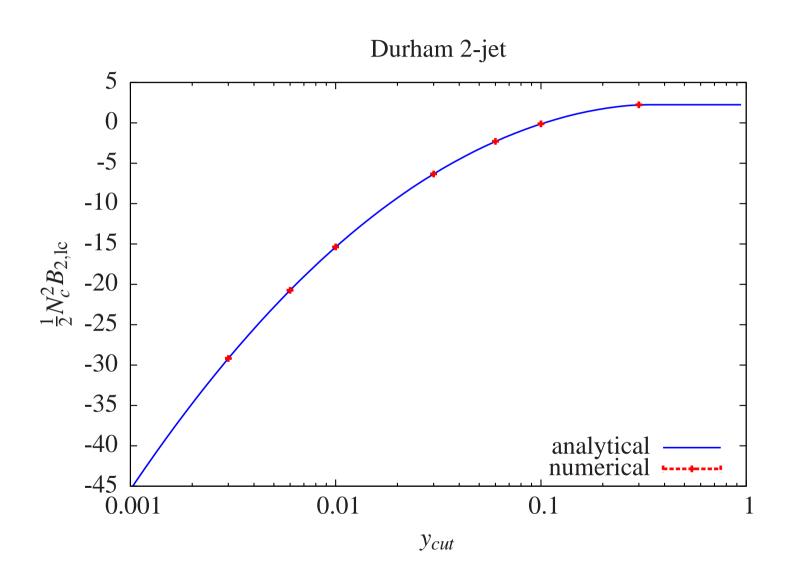
Results for n = 5 have been obtained recently.

R. Frederix, S. Frixione, K. Melnikov and G. Zanderighi, (arXiv:1008.5313).

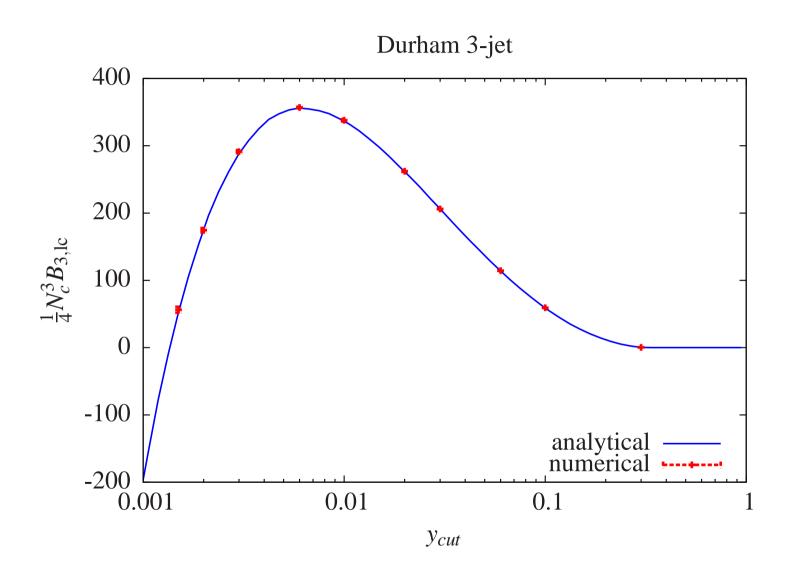
Jets are defined by the Durham jet algorithm.

In the program all parts work for arbitrary n. CPU time scales polynomially with n.

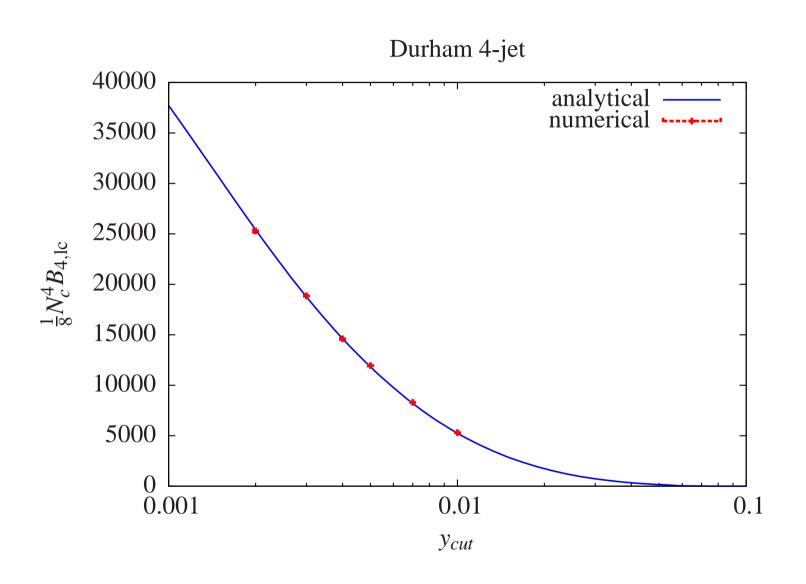
# **Durham 2-jet rate**



# **Durham 3-jet rate**



# **Durham 4-jet rate**



### Durham 5-, 6- and 7-jet rate

Perturbative expansion of the jet-rates:

$$rac{oldsymbol{\sigma}_{n- ext{jet}}}{oldsymbol{\sigma}_0} \quad = \quad \left(rac{lpha_s}{2\pi}
ight)^{n-2} A_n + \left(rac{lpha_s}{2\pi}
ight)^{n-1} B_n + \mathcal{O}(lpha_s^n),$$

Leading-colour coefficient:

$$A_n = N_c \left(\frac{N_c}{2}\right)^{n-2} \left[A_{n,lc} + O\left(\frac{1}{N_c}\right)\right], \qquad B_n = N_c \left(\frac{N_c}{2}\right)^{n-1} \left[B_{n,lc} + O\left(\frac{1}{N_c}\right)\right].$$

Results for five, six and seven jets for the jet parameter  $y_{cut} = 0.0006$ :

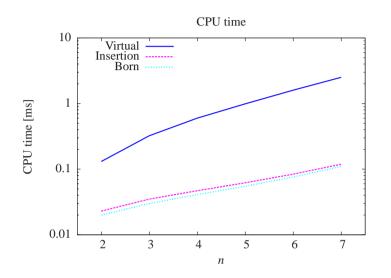
$$\frac{N_c^4}{8}A_{5,lc} = (2.4764 \pm 0.0002) \cdot 10^4, \qquad \frac{N_c^5}{16}B_{5,lc} = (1.84 \pm 0.15) \cdot 10^6, 
\frac{N_c^5}{16}A_{6,lc} = (2.874 \pm 0.002) \cdot 10^5, \qquad \frac{N_c^6}{32}B_{6,lc} = (3.88 \pm 0.18) \cdot 10^7, 
\frac{N_c^6}{32}A_{7,lc} = (2.49 \pm 0.08) \cdot 10^6, \qquad \frac{N_c^7}{64}B_{7,lc} = (5.4 \pm 0.3) \cdot 10^8.$$

First calculation of a physical observable involving a one-loop eight-point function!

## **CPU** scaling behaviour

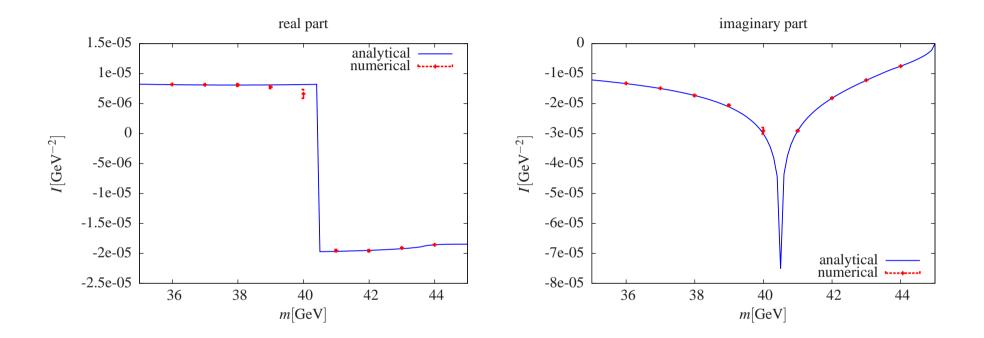
Scaling of the CPU time for one evaluation of the integrand (Born, virtual, insertion) with the number of external particles:

CPU time  $\sim n^4$ 



- *n*<sup>4</sup>-behaviour from recurrence relations
- helicity summation replaced by smooth integration over random polarisations
- Real part: Extension of the dipole formalism to random polarisations
   D. Götz, Ch. Schwan and S.W., '12

## **Extension to massive particles**



Comparison of the results obtained by Monte Carlo integration with the analytical results in the vicinity of a threshold.

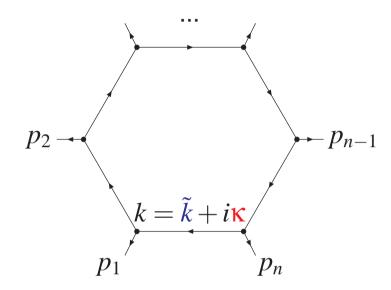
S. Becker and S.W., '12

## **Extension to higher orders**

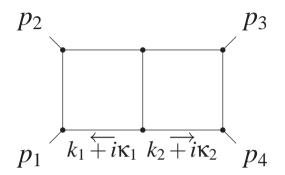
- Subtraction terms
- Contour deformation

$$\int \frac{d^4k}{(2\pi)^4} f(k) = \int \frac{d^4\tilde{k}}{(2\pi)^4} \left| \frac{\partial k^{\mu}}{\partial \tilde{k}^{\nu}} \right| f(k(\tilde{k}))$$

κ vanishes whenever one loop momentum becomes soft.



## **Beyond one-loop**

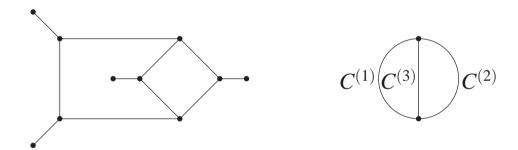


We have:

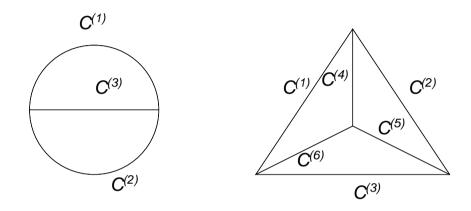
- 2 independent loop momenta
- 3 inequivalent cycles

## **Chain diagrams**

The momenta of the propagators in the same chain differ only by a linear combination of the external momenta.



## Two and three loop chain diagrams

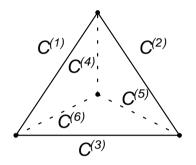


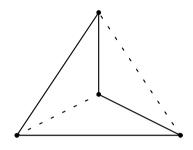
 $\kappa_i$  obtained as the sum of all deformation vectors for cycles containing propagator *i*.

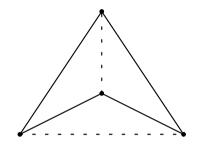
Two-loop example:

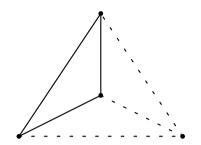
$$\kappa_1 = \kappa^{(12)} + \kappa^{(13)},$$
 $\kappa_2 = \kappa^{(12)} + \kappa^{(23)},$ 

## **Three loops**









$$\kappa_1 = \kappa^{(123)} + \kappa^{(146)} + \kappa^{(1256)} + \kappa^{(1345)},$$

$$\kappa_2 = \kappa^{(123)} + \kappa^{(245)} + \kappa^{(1256)} + \kappa^{(2346)},$$

$$\kappa_3 = \kappa^{(123)} + \kappa^{(356)} + \kappa^{(1345)} + \kappa^{(2346)}.$$

### **Verification and results**

Comparison with analytical result (no internal masses, external legs off-shell):

- two- and three-loop propagator corrections
- two- and three-loop vertex functions (planar and non-planar)
- ladder diagrams (double box, triple box)

### In addition:

• Two-loop six-point functions

### Conclusions

- Numerical method for the computation of NLO corrections
  - Local subtraction terms for ultraviolet, soft and collinear divergences
  - Contour deformation
- First results for jet production in electron-positron annihilation
- More results on LHC processes to come
- Generalisation to higher orders