First steps towards WHIZARD + NLO

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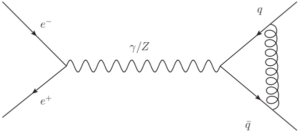
A Textbook Example

Consider the process $e^+e^- \to u\bar{u}$.
Task: Compute the $\mathcal{O}(\alpha_s)$-contributions to the cross section.
So we write down:



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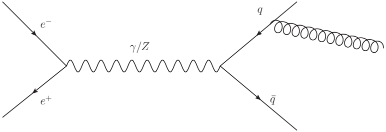
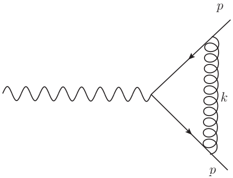


,...

Problem: Matrix elements are divergent for small k!



$$\sim \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \frac{(\not{p} - \not{k})\gamma^\mu(\not{p} + \not{k})}{(p-k)^2(p+k)^2} \supset \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^6}$$

A Textbook Example

Standard approach: Dimensional Regularisation: Perform integration in $d = 4 - 2\varepsilon$ dimensions.
This leads to:

$$\sigma_{\text{virt}} \sim \frac{\alpha_s}{2\pi} \cdot \sigma_{\text{LO}} \cdot C_F \cdot \left(-\frac{2}{\varepsilon^2} - \frac{3}{\varepsilon} - 8 \right),$$

and

$$\sigma_{\text{real}} \sim \frac{\alpha_s}{2\pi} \cdot \sigma_{\text{LO}} \cdot C_F \cdot \left(\frac{2}{\varepsilon^2} + \frac{3}{\varepsilon} + \frac{19}{2} \right).$$

Thus, the total cross section is

$$\sigma_{\text{NLO}} = \sigma_{\text{virt}} + \sigma_{\text{real}} = \sigma_{\text{LO}} \cdot \frac{\alpha_s}{\pi}$$

KLN-Theorem (1964)

The sum of virtual and real amplitudes is finite

Subtraction of Divergences

KLN theorem not valid for event generator:

- Dim. Regularisation works in an abritrary (complex) number of dimensions.
- MC Integration requires explicitly constructed phase space $\rightarrow$ The computer is confined to four dimensions!

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Solution:

Create subtraction terms $\mathcal{C}$ which cancel the divergences of $\mathcal{R}$ and $\mathcal{V}$ and compute

$$\sigma^{\mathrm{NLO}} = \underbrace{\int_{n+1} \left(d\sigma^R - d\sigma^C\right)}_{\text{finite}} + \underbrace{\int_{n+1} d\sigma^C + \int_n d\sigma^V}_{\text{finite}}$$

Common Subtraction Schemes

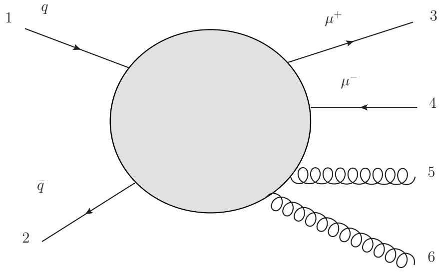
The most frequently used subtraction schemes ared

- Catani Seymour [S. Catani and M. H. Seymour, hep-ph/9605323]
  Uses dipole splitting functions

  $$\mathcal{D}_{ij,k} = \langle 1, \ldots, \tilde{ij}, \ldots, \tilde{k}, \ldots, n | 1, \ldots, \tilde{ij}, \ldots, \tilde{k}, \ldots, n \rangle \otimes V_{ij,k}$$

  Implemented e.g. in HERWIG++, SHERPA
- FKS [R. Frederix, S. Frixione, F. Maltoni, T. Stelzer, arXiv:0908.4272]
  Uses phase-space mappings and plus-distributions
  Implemented e.g. in POWHEG-BOX, MG5_aMC, WHIZARD
- Nagy-Soper [C. Chung, M. Krämer, T. Robens, arXiv:1012.4948]
  Uses fully spin- and color-correlated splitting functions of improved parton shower [Z. Nagy and E. Soper, arXiv:0706.0017]
  Implemented e.g. in HELAC + DEDUCTOR

FKS subtraction



i) Find all tuples of particle indices which can give rise to a singularity, e.g.

$$\mathcal{I} = \{(1,5),(1,6),(2,5),(2,6),(5,6)\}$$

ii) Partition the phase space:

$$1 = \sum_{\alpha \in \mathcal{I}} S_\alpha(\Phi),$$

such that the real matrix element $\mathcal{R}$

$$\mathcal{R} = \sum_{\alpha \in \mathcal{I}} \mathcal{R}_\alpha, \qquad \underbrace{\mathcal{R}_\alpha}_{\text{Singular only for one tuple!}} = \mathcal{R} S_\alpha$$

iii) Add subtraction terms for each singular region.

Constructing Subtraction Terms

Real subtraction: Factorization in the soft and collinear limit

$$|\mathcal{A}^{(n+1)}(\Phi_{n+1})|^2 \to \mathcal{D}_{\mathcal{I}} \otimes |\mathcal{A}^{(n)}(\Phi_n)|^2$$

$\otimes$: Convolution over spin and color.

Soft subtraction involves color-correlated matrix elements:

$$\mathcal{B}_{kl} \sim -\sum_{\substack{\text{color}\\ \text{spin}}} \mathcal{A}^{(n)} \vec{\mathcal{Q}}(\mathcal{I}_k) \cdot \vec{\mathcal{Q}}(\mathcal{I}_l) \mathcal{A}^{(n)*},$$

with

$$\vec{\mathcal{Q}}(\mathcal{I}) = \{t^a\}_{a=1}^{8}, \{-t^{aT}\}_{a=1}^{8}, \{T^a\}_{a=1}^{8}$$

Collinear subtraction involves spin-correlated matrix elements:

$$\mathcal{B}_{+-} \sim Re\left\{ \frac{\langle k_{\text{em}} k_{\text{rad}} \rangle}{[k_{\text{em}} k_{\text{rad}}]} \sum_{\substack{\text{color}\\ \text{spin}}} \mathcal{A}_{+}^{(n)} \mathcal{A}_{-}^{(n)*} \right\}$$

Constructing Subtraction Terms

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Virtual subtraction: Same structure

$$|\mathcal{M}_n^{virt}|^2 \to \mathcal{V}_{\mathcal{I}} \otimes |\mathcal{M}_n|^2, \quad \mathcal{V}_{\mathcal{I}} = \int d\Phi_{\text{rad}} \mathcal{D}_{\mathcal{I}}$$

What an automated NLO (+FKS) calculation must do

- $N+1$-particle flavor configurations must be constructed from N-particle configurations
- The set of singular regions, $\mathcal{I}$ must be generated and mappings $\mathcal{S}_\alpha$ computed
- Appropriate $N+1$-particle phase spaces must be generated
- In addition to the Born matrix element, real and virtual amplitudes, as well as color- and spin-correlated Born matrix elements, must be computed.
- The above ingredients should be combined in a parton shower matching or merging procedure
- Ideally, user responsibility is zero

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- $N+1$-particle flavor configurations must be constructed from N-particle configurations ✓
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- The above ingredients should be combined in a parton shower matching or merging procedure✓
- Ideally, user responsibility is zero✓

NLO in WHIZARD

Phase space:

- Construct Born kinematics as usual
- Radiation phase space parameterized through $\xi = \frac{2E_{\rm rad}}{\sqrt{s}}$, $y = \cos\theta$ and ϕ
  $\rightarrow$ Construct real phase space for each emitter

Integration:

- Individual component for Born, real-subtracted and virtual-subtracted matrix elements
- Integration either performed separately for each component or over the sum of all

Matrix elements:

- Virtual amplitudes computed by GoSam [G. Cullen et.al., arXiv:1404.7096]
- $\mathcal{B}_{kl}$, $\mathcal{B}_{+-}$ computed by GoSam
- $\mathcal{B}_{kl}$: For some processes with WHIZARD /O'Mega

Possible Constellations:

	$\mathcal{R}_{\rm tree}$	$\mathcal{B}_{kl}$	$\mathcal{B}_{+-}$	$\mathcal{V}$
O'Mega	🟡	🟡	🔴	🔴
GoSam	🟢	🟢	🟢	🟢

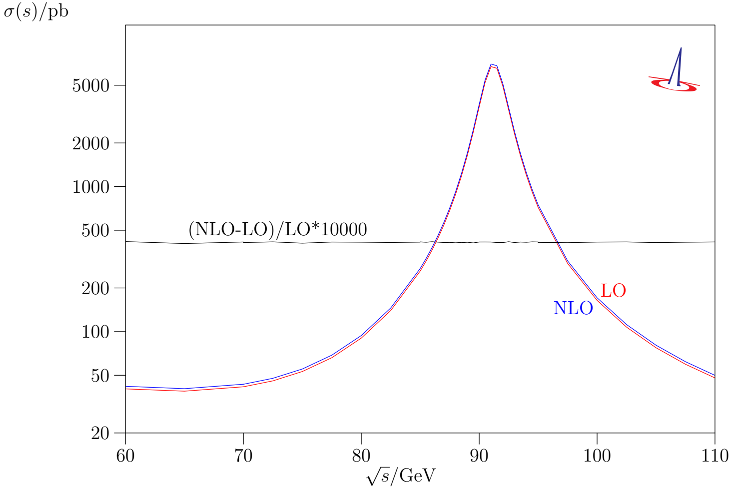
🟢: Computation possible
🟡: Computation possible for some processes
🔴: Computation not possible (so far)

Proof of Concept - Total Cross Sections

Simplest Process: $e^+e^- \to q\bar{q}$, with $(\sigma^{\text{NLO}} - \sigma^{\text{LO}})/\sigma^{\text{LO}} = \alpha_s/\pi$ for massless quarks.

$\to$ Benchmark Process!

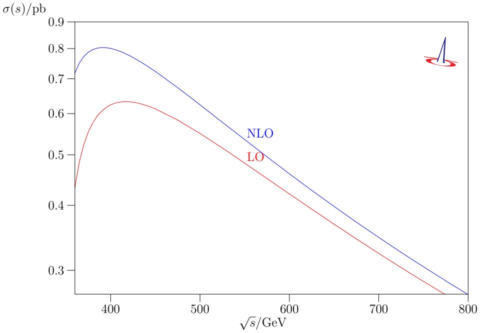
Total cross section for the process $e^+e^- \to u\bar{u}$, α_s fixed



Proof of Concept - Total Cross Sections

- More complicated processes have been evaluated:
  - $e^+e^- \to t\bar{t}$
  - $e^+e^- \to q\bar{q}l^+l^-$
  - $e^+e^- \to q\bar{q}\nu_l l^+$
  - $e^+e^- \to q\bar{q}g$
- Cross-checks with MadGraph5_aMC@NLO passed
- Feature is contained in the current release version 2.2.5 of `WHIZARD`

Total cross section for the process
$e^+e^- \to t\bar{t}, m_t = 173\text{GeV}$



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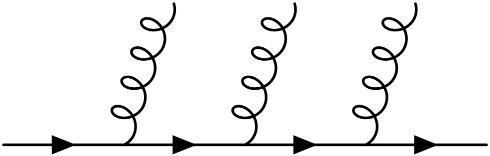
The POWHEG approach

Problem: Soft gluon emissions before a hard emission are $\mathcal{O}(1)$!



- Reason: $|\mathcal{M}_{\mathrm{soft}}|^2 \sim \frac{1}{k_T^2} \to \log \frac{p_T^{\max}}{p_T^{\min}}$ after phase-space integration
  $\to$ Large logarithms!
- Smallness of α_s is compensated by this logarithm: $\alpha_s \log \frac{p_T^{\max}}{p_T^{\min}} \sim 1$

$\to$ ME + Parton Shower must take this configurations into account.
POWHEG [P. Nason, hep-ph/0409146] : Hardest Emission First!

The POWHEG approach

POWHEG matching proceeds in two steps:

1. Generate events according to the distribution

$$d\sigma = \bar{B}(\Phi_n)\left[\Delta_R^{\mathrm{NLO}}(p_T^{\mathrm{min}}) + \Delta_R^{\mathrm{NLO}}(k_T)\frac{R(\Phi_{n+1})}{B(\Phi_n)}d\Phi_{\mathrm{rad}}\right],$$

   with the complete NLO matrix element

$$\bar{B}(\Phi_n) = B(\Phi_n) + V(\Phi_n) + \int d\Phi_{\mathrm{rad}} R(\Phi_{n+1})$$

   and the modified Sudakov form factor

$$\Delta_R^{\mathrm{NLO}}(p_T) = \exp\left[-\int d\Phi_{\mathrm{rad}}\frac{R(\Phi_{n+1})}{B(\Phi_n)}\theta(k_T(\Phi_{n+1}) - p_T)\right],$$

2. Generation of the hardest emission occurs at the scale p_T^{max}. Shower the generated events, imposing a veto $p_T^{\mathrm{max}} > p_T$ for all emissions

Positive Weights

Consider the POWHEG formula

$$d\sigma = \bar{B}(\Phi_n)\left[\Delta_R^{\mathrm{NLO}}(p_T^{\mathrm{min}}) + \Delta_R^{\mathrm{NLO}}(k_T)\frac{R(\Phi_{n+1})}{B(\Phi_n)}d\Phi_{\mathrm{rad}}\right]$$

Sign of Weights:

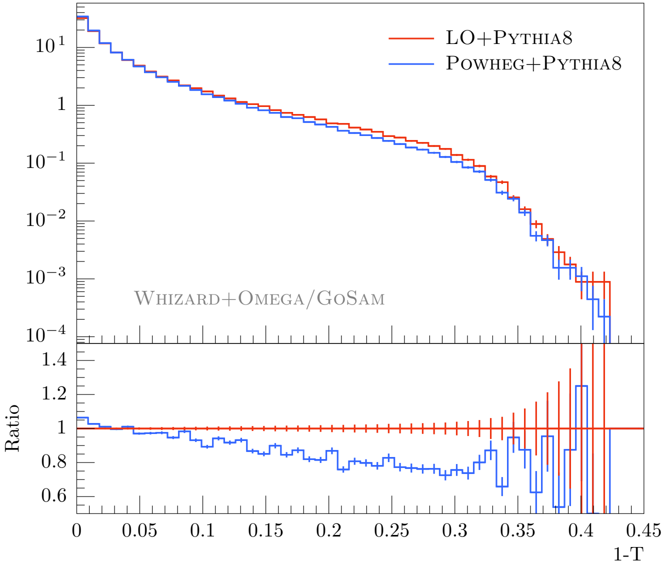
- Determined by sign of $\bar{B}$
- $\bar{B} < 0$ if the virtual and real terms are larger in magnitude than the Born contribution.
  $\rightarrow$ should not happen in perturbative regions!
- Therefore, $\bar{B} > 0$ for all events

POWHEG matching produces events with positive weights

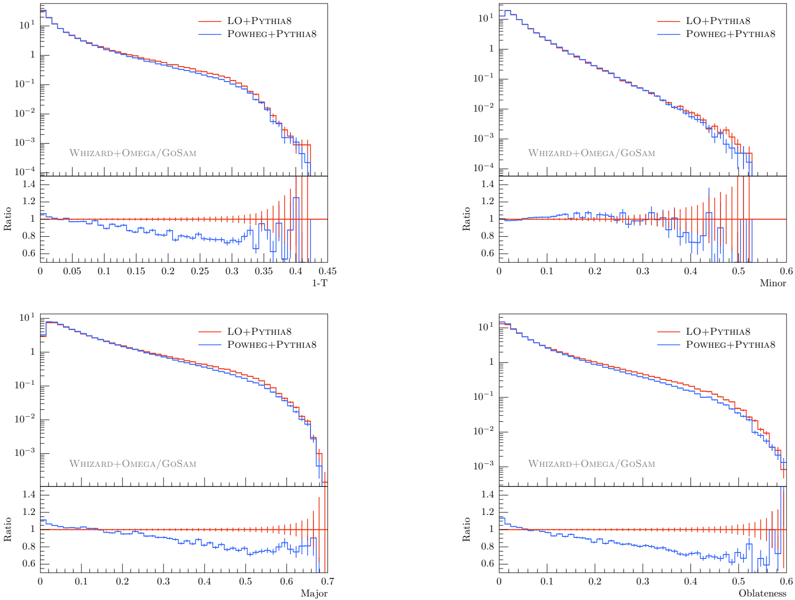
(POWHEG $=$ **Po**sitive **W**eight **H**ardest **E**mission **G**enerator)
Very convenient feature for performance of experimental applications

$e^+e^- \to u\bar{u}$ at NLO matched to Parton Shower

`WHIZARD` now has its own implementation of the POWHEG method



$e^+e^- \to u\bar{u}$ at NLO matched to Parton Shower



More on WHIZARD + POWHEG on Tuesday! → Bijan Chokoufé

Conclusion & Outlook

- NLO-calculations for final-state QCD corrections are currently an experimental feature available in the current release
- Experimental POWHEG matching is present and will be added to the next release of `WHIZARD`

Plans for the future

- Validation of results for higher particle multiplicities
- NLO-treatment of hadron collisions; Electroweak corrections
- Modular structure of `WHIZARD` could allow for the inclusion of other subtraction/matching schemes (MC@NLO, Nagy-Soper?)

What are your wishes?

Which processes are you especially interested in? How would you like to control NLO-computations?

SINDARIN - Example

Scripting INtegration, Data Analysis, Results display and INterfaces

```
#Sindarin script for the production of quarks in electron-positron
collisions at NLO
#Set some particle properties, process flags etc.
mtop = 137.1 GeV
wtop = 0 # Zero top width for on-shell production
.....
process lo = E1, e1 => t, T #Define processes
process nlo1 = E1, e1 => t, T {nlo_calculation=''Full''}
# Define plots
plot lineshape_lo {x_min = 380 GeV x_max = 800 GeV}
plot lineshape_nlo1 {x_min = 380 GeV x_max = 800 GeV}
# Loop over CMS energies and record xsection
scan sqrts = ((360 GeV => 450 GeV /+ 5 GeV),
(450 GeV => 800 GeV /+ 25 GeV))
integrate (lo) iterations=5:5000:''gw''
record lineshape_lo (sqrts, integral (lo) / 1000)
integrate (nlo1) {iterations=5:5000:''gw''}
record lineshape_nlo1 (sqrts, integral (nlo1) / 1000)
....(Histogram compilation and plotting options)
```

Available Models

MODEL TYPE	with CKM matrix	trivial CKM
Yukawa test model	---	Test
QED with e, μ, τ, γ	---	QED
QCD with d, u, s, c, b, t, g	---	QCD
Standard Model	SM_CKM	SM
SM with anomalous gauge couplings	SM_ac_CKM	SM_ac
SM with Hgg, $H\gamma\gamma$, $H\mu\mu$	---	SM_Higgs
SM with charge 4/3 top	---	SM_top
SM with anomalous top couplings	---	SM_top_anom
SM with K matrix	---	SM_KM
MSSM	MSSM_CKM	MSSM
MSSM with gravitinos	---	MSSM_Grav
NMSSM	NMSSM_CKM	NMSSM
extended SUSY models	---	PSSSM
Littlest Higgs	---	Littlest
Littlest Higgs with ungauged $U(1)$	---	Littlest_Eta
Littlest Higgs with T parity	---	Littlest_Tpar
Simplest Little Higgs (anomaly-free)	---	Simplest
Simplest Little Higgs (universal)	---	Simplest_univ
SM with graviton	---	Xdim
UED	---	UED
SM with Z'	---	Zprime
"SQED" with gravitino	---	GravTest
Augmentable SM template	---	Template

Observables

The **Thrust** observable is defined as

$$T = \max_{|\vec{n}|=1} \frac{\sum_i |\vec{p}_i \cdot \vec{n}|}{\sum_i |\vec{p}_i|} \in [1/2, 1]$$

- Two back-to-back jets: $T = 1$
- Spherically symmetric distribution: $T = \frac{1}{2}$

$\rightarrow T \neq 1$ implies deviation from 2-jet structure
Further observables

$$T_{major} = \max_{|\vec{n}'|=1, \vec{n}'\vec{n}=0} \frac{\sum_i |\vec{p}_i \cdot \vec{n}'|}{\sum_i |\vec{p}_i|},$$

$$T_{minor} = \frac{\sum_i |\vec{p}_i \cdot \vec{n}''|}{\sum_i |\vec{p}_i|}, \quad \text{with} \quad \tilde{\mathrm{n}}''\tilde{\mathrm{n}} = \tilde{\mathrm{n}}''\tilde{\mathrm{n}}' = 0$$

$$\text{Oblateness} = T_{major} - T_{minor}$$

References

POWHEG

[1] P. Nason, *"A New Method for Combining NLO QCD with Shower Monte Carlo Algorithms"*, JHEP **0411**, hep-ph/0409146

[2] S. Frixione et. al., *"Matching NLO QCD Computations with Parton Shower Simulations: the POWHEG Method"*, JHEP 0711, arXiv:0709.2092.

[3] S. Alioli et. al., *"A general Framework for implementing NLO Calculations in Shower Monte Carlo Programs: the POWHEG BOX"*, JHEP 1006, arXiv:1002.2581

FKS

[4] S. Frixione, *"A General Approach to Jet Cross Sections in QCD"*, Nucl.Phys. B507, hep-ph/9706545.

[5] R. Frederix et. al. *"Automation of NLO computations in QCD: The FKS subtraction"*, JHEP 0910, arXiv:0908.4272