Techniques and phenomenology of cutting-edge higher-order calculations for LHC processes

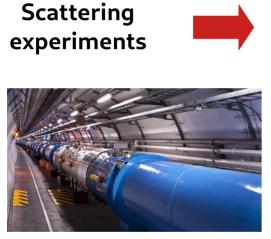
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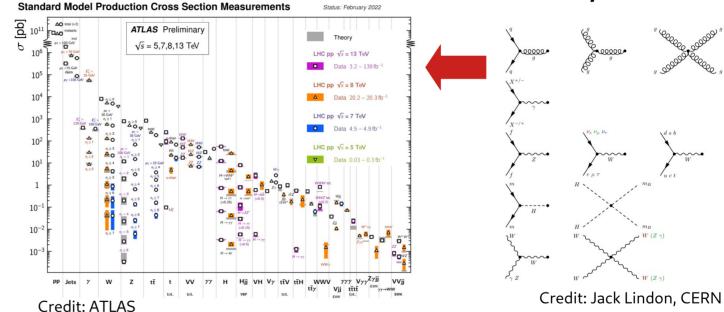
Presented research received funding from: LEVERHULME TRUST______

- Introduction
- Sector-improved residue subtraction
- Two-loop five-point amplitudes
- → Pheno @ LHC:
 - → Three-jet production through NNLO QCD→ HighTEA
- Summary and Outlook

What are the fundamental building blocks of matter?

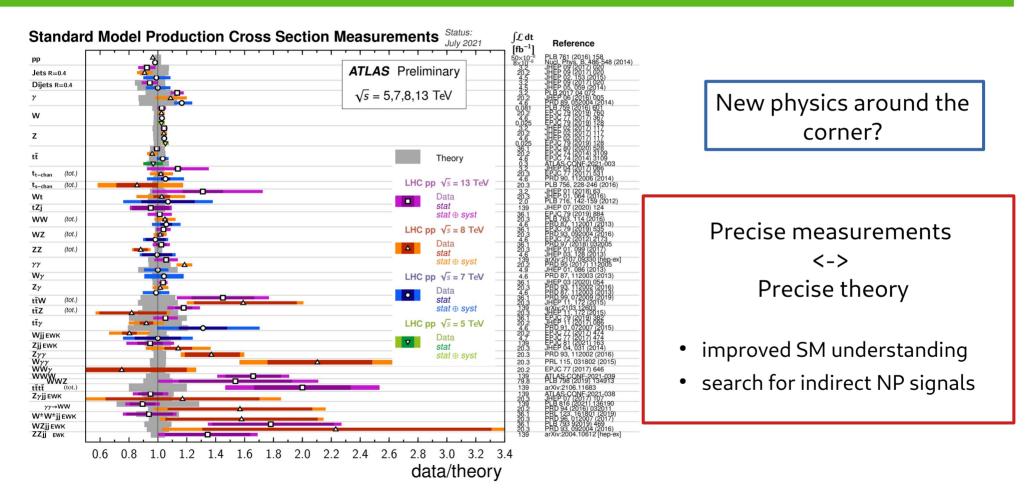


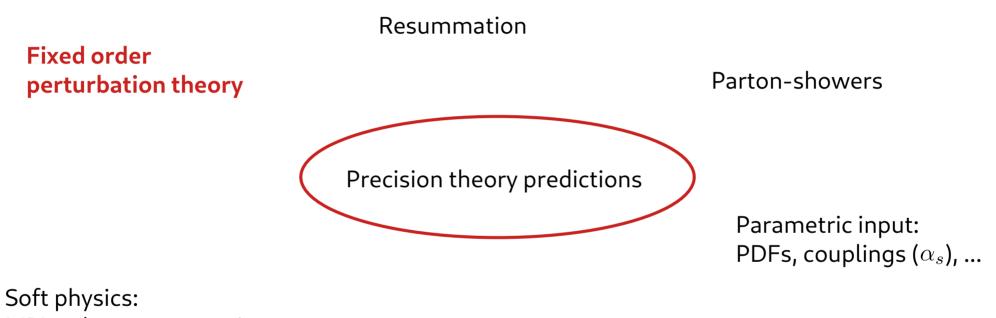
Credit: CERN



Theory/Model

SM measurements at the LHC



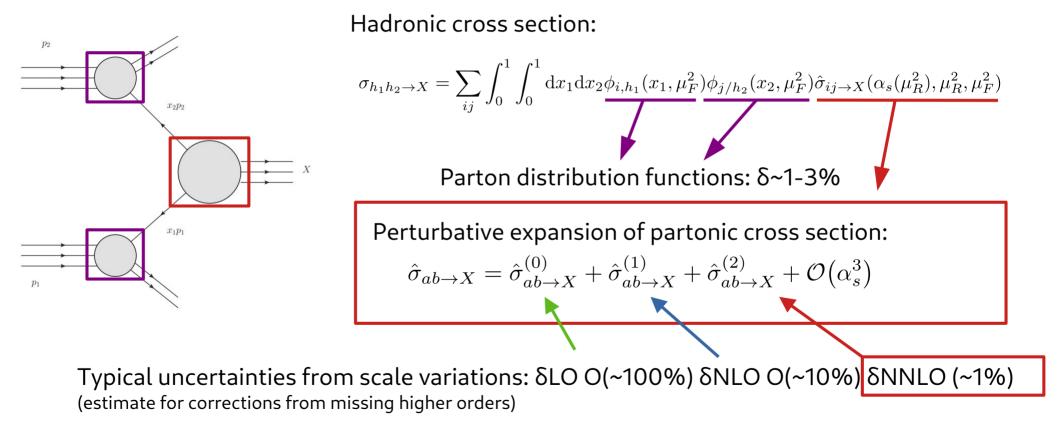


MPI, colour reconnection,

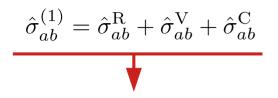
Fragmentation/hadronisation

...

Perturbative QCD



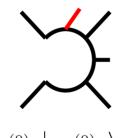
Next-to-leading order case



KLN theorem sum is finite for sufficiently inclusive observables and regularization scheme independent

Each term separately infrared (IR) divergent:

Real corrections:



 $\hat{\sigma}_{ab}^{\mathrm{R}} = \frac{1}{2\hat{s}} \int \mathrm{d}\Phi_{n+1} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(0)} \right\rangle \mathrm{F}_{n+1}$

Phasespace integration over unresolved configurations

Collinear factorization: $\hat{\sigma}_{ab}^{C} = (\text{single convolution}) F_n$

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Virtual corrections:

$$\hat{\sigma}_{ab}^{V} = \frac{1}{2\hat{s}} \int d\Phi_n 2\text{Re} \left\langle \mathcal{M}_n^{(0)} \middle| \mathcal{M}_n^{(1)} \right\rangle F_n$$

Integration over loop-momentum

Central idea: Divergences arise from infrared (IR, soft/collinear) limits → Factorization!

Slicing

$$\hat{\sigma}_{ab}^{R} = \frac{1}{2\hat{s}} \int_{\delta(\Phi) \ge \delta_{c}} d\Phi_{n+1} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(0)} \right\rangle F_{n+1} + \frac{1}{2\hat{s}} \int_{\delta(\Phi) < \delta_{c}} d\Phi_{n+1} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(0)} \right\rangle F_{n+1} \\ \approx \frac{1}{2\hat{s}} \int_{\delta(\Phi) \ge \delta_{c}} d\Phi_{n+1} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(0)} \right\rangle F_{n+1} + \frac{1}{2\hat{s}} \int d\Phi_{n} \, \tilde{M}(\delta_{c}) F_{n} + \mathcal{O}(\delta_{c})$$

- Conceptually simple
- Recycling of lower computations
- Non-local cancellations/power-corrections
 → computationally expensive

Subtraction

$$\frac{1}{2\hat{s}} \int \mathrm{d}\tilde{\Phi}_{n+1} \,\mathcal{S}\mathrm{F}_n = \frac{1}{2\hat{s}} \int \mathrm{d}\Phi_n \,\mathrm{d}\Phi_1 \,\mathcal{S}\mathrm{F}_n$$

Phasespace factorization → momentum mappings

 $\dots + \hat{\sigma}_{ab}^{V} = \text{finite}$

- Conceptually more difficult
- Local subtraction → efficient
- Better numerical stability

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 $\hat{\sigma}_{ab}^{\mathrm{R}} = \frac{1}{2\hat{s}} \int \left(\mathrm{d}\Phi_{n+1} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(0)} \right\rangle \mathrm{F}_{n+1} - \mathrm{d}\tilde{\Phi}_{n+1} \,\mathcal{S}\mathrm{F}_n \right) + \frac{1}{2\hat{s}} \int \mathrm{d}\tilde{\Phi}_{n+1} \,\mathcal{S}\mathrm{F}_n$

Partonic cross section beyond NLO

$$\hat{\sigma}_{ab}^{(2)} = \hat{\sigma}_{ab}^{\text{VV}} + \hat{\sigma}_{ab}^{\text{RV}} + \hat{\sigma}_{ab}^{\text{RR}} + \hat{\sigma}_{ab}^{\text{C2}} + \hat{\sigma}_{ab}^{\text{C1}}$$

$$\textbf{Real-Real} \qquad \hat{\sigma}_{ab}^{\text{RR}} = \frac{1}{2\hat{s}} \int d\Phi_{n+2} \left\langle \mathcal{M}_{n+2}^{(0)} \middle| \mathcal{M}_{n+2}^{(0)} \right\rangle \mathbf{F}_{n+2}$$

$$\textbf{Real-Virtual} \qquad \hat{\sigma}_{ab}^{\text{RV}} = \frac{1}{2\hat{s}} \int d\Phi_{n+1} 2\text{Re} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(1)} \right\rangle \mathbf{F}_{n+1}$$

$$\textbf{Virtual-Virtual} \qquad \hat{\sigma}_{ab}^{\text{VV}} = \frac{1}{2\hat{s}} \int d\Phi_n \left(2\text{Re} \left\langle \mathcal{M}_n^{(0)} \middle| \mathcal{M}_n^{(2)} \right\rangle + \left\langle \mathcal{M}_n^{(1)} \middle| \mathcal{M}_n^{(1)} \right\rangle \right) \mathbf{F}_n$$

$$\hat{\sigma}_{ab}^{\text{C2}} = (\text{double convolution}) \mathbf{F}_n \qquad \hat{\sigma}_{ab}^{\text{C1}} = (\text{single convolution}) \mathbf{F}_{n+1}$$

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Central idea: Divergences arise from infrared (IR, soft/collinear) limits → Factorization!

Slicing

qT-slicing [Catain'07], N-jettiness slicing [Gaunt'15/Boughezal'15]

- Conceptually simple
- Recycling of lower computations
- Non-local cancellations/power-corrections
 → computationally expensive

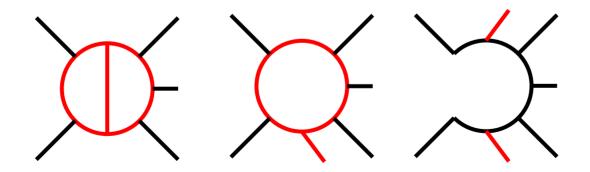
Subtraction

- Conceptually more difficult
- Local subtraction → efficient
- Better numerical stability

Antenna [Gehrmann'05-'08], Colorful [DelDuca'05-'15], Projetction [Cacciari'15], Geometric [Herzog'18], Unsubtraction [Aguilera-Verdugo'19], Nested collinear [Caola'17], Sector-improved residue subtraction [Czakon'10-'14'19]

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Sector-improved residue subtraction



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Considering working in CDR:

- → Virtuals are usually done in this regularization: $\hat{\sigma}_{ab}^{VV} = \sum_{i=-4}^{\circ} c_i \epsilon^i + \mathcal{O}(\epsilon)$
- → Can we write the real radiation as such expansion?
 - → Difficult integrals, analytical impractical (except very simple observables)!
 - \rightarrow Numerics not possible, integrals are divergent $\rightarrow \epsilon$ -poles!

How to extract these poles? → Sector decomposition!

Divide and conquer the phase space:

Divide and conquer the phase space

- Each $S_{i,k}$ (NLO), $S_{ij,k}/S_{i,k;j,l}$ (NNLO) has simpler divergences:
 - Soft limits of partons i and j
 - Collinear w.r.t partons k (and l) of partons i and j

$$S_{i,k} = \frac{1}{D_1 d_{i,k}} \quad D_1 = \sum_{ik} \frac{1}{d_{i,k}} \quad d_{i,k} = \frac{E_i}{\sqrt{s}} (1 - \cos \theta_{ik})$$

• Parametrization w.r.t. reference parton makes divergences explicit

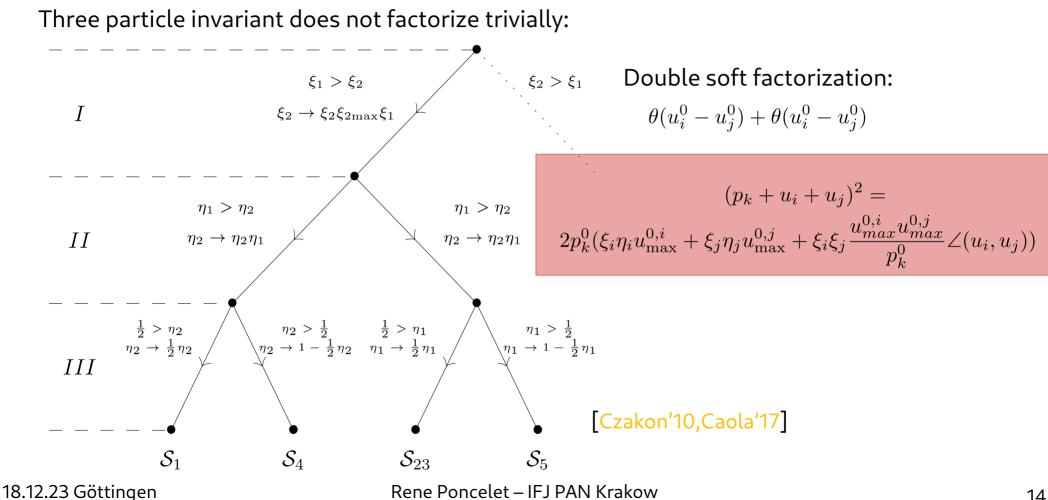
$$\hat{\eta}_i = \frac{1}{2}(1 - \cos\theta_{ik}) \in [0, 1]$$
 $\hat{\xi}_i = \frac{u_i^0}{u_{\max}^0} \in [0, 1]$

• Example: Splitting function

$$\sim \frac{1}{s_{ik}} P(z)$$
 $s_{ik} = (p_i + p_k)^2 = 2p_k^0 u_{\max}^0 \xi_i \eta_i$ $\sim \frac{1}{\eta_i \xi_i}$

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Sector decomposition II – triple collinear factorization



Sector decomposition III

Factorized singular limits in each sector:

$$\frac{1}{2\hat{s}} \int d\Phi_{n+2} \mathcal{S}_{kl,m} \left\langle \mathcal{M}_{n+2}^{(0)} \middle| \mathcal{M}_{n+2}^{(0)} \right\rangle F_{n+2} = \sum_{\text{sub-sec.}} \int d\Phi_n \prod dx_i \underbrace{x_i^{-1-b_i\epsilon}}_{\text{singular}} d\tilde{\mu}(\{x_i\}) \underbrace{\prod x_i^{a_i+1} \left\langle \mathcal{M}_{n+2} \middle| \mathcal{M}_{n+2} \right\rangle}_{\text{regular}} F_{n+2}$$

$$x_i \in \{\eta_1, \xi_1, \eta_2, \xi_2\}$$

Regularization of divergences:



Finite NNLO cross section

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C++ framework

- Formulation allows efficient algorithmic implementation → STRIPPER
- High degree of automation:
 - Partonic processes (taking into account all symmetries)
 - Sectors and subtraction terms
 - Interfaces to Matrix-element providers + O(100) hardcoded: AvH, OpenLoops, Recola, NJET, HardCoded

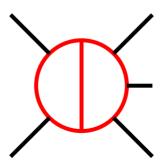
→ In practice: Only two-loop matrix elements required

- **Broad range of applications** through additional facilities:
 - Narrow-Width & Double-Pole Approximation
 - Fragmentation
 - Polarised intermediate massive bosons
 - (Partial) Unweighting → Event generation for **HighTEA**
 - Interfaces: FastNLO, FastJet

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Two-loop five-point amplitudes

Massless: [Chawdry'19'20'21] (3A+2j,2A+3j) [Abreu'20'21] (3A+2j,5j) [Agarwal'21] (2A+3j) [Badger'21'23] (5j,gggAA,jjjjA)

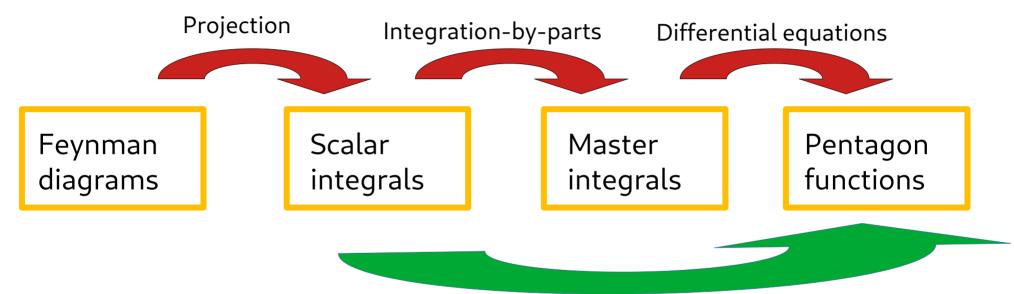


1 external mass: [Abreu'21] (W+4j) [Badger'21'22] (Hqqgg,W4q,Wajjj) [Hartanto'22] (W4q)

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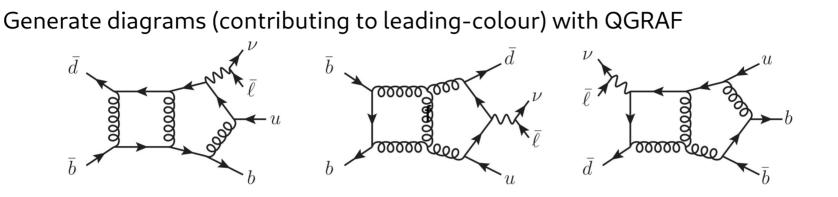
Overview

Old school approach:



Automated framework using finite fields to avoid expression swell based on FiniteFlow [Peraro'19]

Projection to scalar integrals



Factorizing decay: $A_6^{(L)} = A_5^{(L)\mu} D_\mu P$ $M_6^{2(L)} = \sum_{\text{spin}} A_6^{(0)^*} A_6^{(L)} = M_5^{(L)\mu\nu} D_{\mu\nu} |P|^2$

Projection on scalar functions (FORM+Mathematica): \rightarrow anti-commuting γ_5 + Larin prescription $M_5^{(L)\mu\nu} = \sum_{i=1}^{16} a_i^{(L)} v_i^{\mu\nu}$

 $a_i^{(L),p} = \sum c_{j,i}(\{p\},\epsilon)\mathcal{I}(\{p\},\epsilon)$

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 $a_i^{(L)} = a_i^{(L),\text{even}} + \text{tr}_5 a_i^{(L),\text{odd}}$

$$a_i^{(L),p} = \sum_i c_{j,i}(\{p\}, \epsilon) \mathcal{I}(\{p\}, \epsilon) \longrightarrow \text{ prohibitively large number of integrals}$$

$$\mathcal{I}_i(\{p\}, \epsilon) \equiv \mathcal{I}(\vec{n_i}, \{p\}, \epsilon) = \int \frac{\mathrm{d}^d k_1}{(2\pi)^d} \frac{\mathrm{d}^d k_2}{(2\pi)^d} \prod_{k=1}^{11} D_k^{-n_{i,k}}(\{p\}, \{k\})$$

Integration-By-Parts identities connect different integrals → system of equations → only a small number of independent "master" integrals

$$0 = \int \frac{\mathrm{d}^d k_1}{(2\pi)^d} \frac{\mathrm{d}^d k_2}{(2\pi)^d} l_\mu \frac{\partial}{\partial l^\mu} \prod_{k=1}^{11} D_k^{-n_{i,k}}(\{p\},\{k\}) \quad \text{with} \quad l \in \{p\} \cap \{k\}$$

LiteRed (+ Finite Fields)

$$a_i^{(L),p} = \sum_i d_{j,i}(\{p\},\epsilon) \operatorname{MI}(\{p\},\epsilon)$$

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Master integrals & finite remainder

Differential Equations: $d\vec{MI} = dA(\{p\}, \epsilon)\vec{MI}$ [Remiddi, 97]Canonical basis: $d\vec{MI} = \epsilon d\tilde{A}(\{p\})\vec{MI}$ [Henn, 13]

Simple iterative solution

$$MI_{i} = \sum_{w} \epsilon^{w} \tilde{MI}_{i}^{w} \text{ with } \tilde{MI}_{i}^{w} = \sum_{j} c_{i,j} m_{j}$$
Chen-iterated integrals
"Pentagon"-functions
[Chicherin, Sotnikov, 20]
[Chicherin, Sotnikov, Zoia, 21]

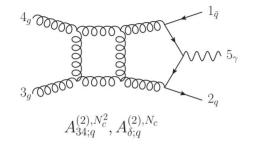
Putting everything together (and removing of IR poles):

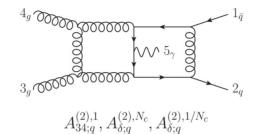
$$f_i^{(L),p} = a_i^{(L),p} - \text{poles}$$
 $f_i^{(L),p} = \sum_j c_{i,j}(\{p\})m_j + \mathcal{O}(\epsilon)$

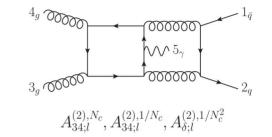
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Reconstruction of Amplitudes

[Badger'21]







New optimizations

- Syzygy's to simplify IBPs
- Exploitation of Q-linear relations
- Denominator Ansaetze
- On-the-fly partial fractioning

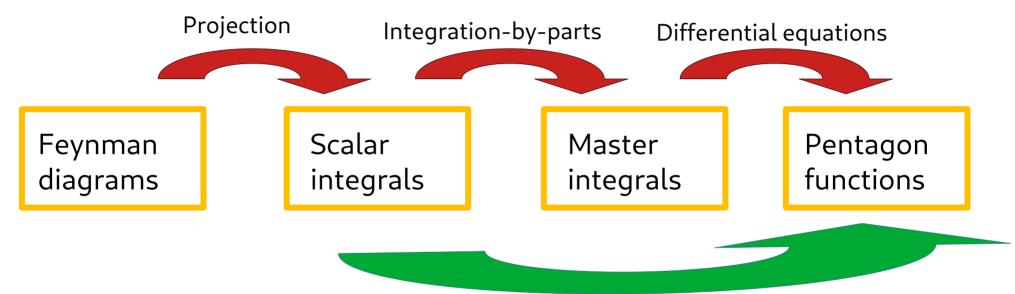
amplitude	helicity	original	stage 1	stage 2	stage 3	stage 4
$A^{(2),1}_{34;q}$	-++-+	94/91	74/71	74/0	22/18	22/0
$A^{(2),1}_{34;q}$	-+-++	93/89	90/86	90/0	24/14	18/0
$A^{(2),1/N_c^2}_{34;q}$	-++-+	90/88	73/71	73/0	23/18	22/0
$A_{34;q}^{(2),1/N_c^2}$	-+-++	90/86	86/82	86/0	24/14	19/0
$A^{(2),1/N_c}_{34;l}$	-+-++	89/82	74/67	73/0	27/14	20/0
$A^{(2),1/N_c}_{34;l}$	-++-+	85/81	61/58	60/0	27/18	20/0
$A^{(2),N^2_c}_{34;q}$	-+-++	58/55	54/51	53/0	20/16	20/0

Massive reduction of complexity

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Overview

Old school approach:



Automated framework using finite fields to avoid expression swell based on FiniteFlow [Peraro'19]

Three-jet production through NNLO QCD

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Multi-jet observables

Test of pQCD and extraction of strong coupling constant NLO theory unc. > experimental unc.

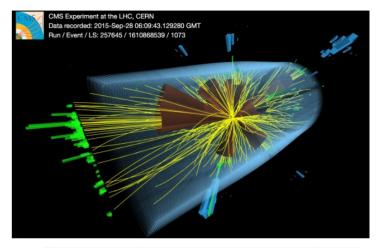
- NNLO QCD needed for precise theory-data comparisons
 → Restricted to two-jet data [Currie'17+later][Czakon'19]
- New NNLO QCD three-jet → access to more observables
 - Jet ratios

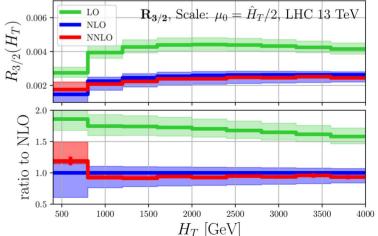
Next-to-Next-to-Leading Order Study of Three-Jet Production at the LHC Czakon, Mitov, **Poncelet** [2106.05331]

$$R^{i}(\mu_{R}, \mu_{F}, \text{PDF}, \alpha_{S,0}) = \frac{\mathrm{d}\sigma_{3}^{i}(\mu_{R}, \mu_{F}, \text{PDF}, \alpha_{S,0})}{\mathrm{d}\sigma_{2}^{i}(\mu_{R}, \mu_{F}, \text{PDF}, \alpha_{S,0})}$$

• Event shapes

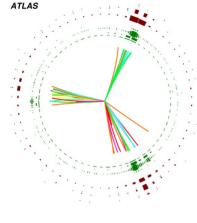
NNLO QCD corrections to event shapes at the LHC Alvarez, Cantero, Czakon, Llorente, Mitov, Poncelet [2301.01086]





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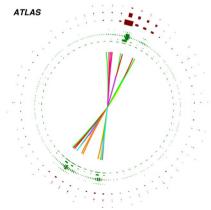
Encoding QCD dynamics in event shapes



Using (global) event information to separate different regimes of QCD event evolution:

- Thrust & Thrust-Minor $T_{\perp} = \frac{\sum_i |\vec{p}_{T,i} \cdot \hat{n}_{\perp}|}{\sum_i |\vec{p}_{T,i}|}$, and $T_m = \frac{\sum_i |\vec{p}_{T,i} \times \hat{n}_{\perp}|}{\sum_i |\vec{p}_{T,i}|}$.
- Energy-energy correlators

$$-\frac{1}{\sigma_2}\frac{\mathrm{d}\sigma}{\mathrm{d}\cos\Delta\phi} = \frac{1}{\sigma_2}\sum_{ij}\int\frac{\mathrm{d}\sigma \, x_{\perp,i}x_{\perp,j}}{\mathrm{d}x_{\perp,i}\mathrm{d}x_{\perp,j}\mathrm{d}\cos\Delta\phi_{ij}}\delta(\cos\Delta\phi - \cos\Delta\phi_{ij})\mathrm{d}x_{\perp,i}\mathrm{d}x_{\perp,j}\mathrm{d}\cos\Delta\phi_{ij}\,,$$

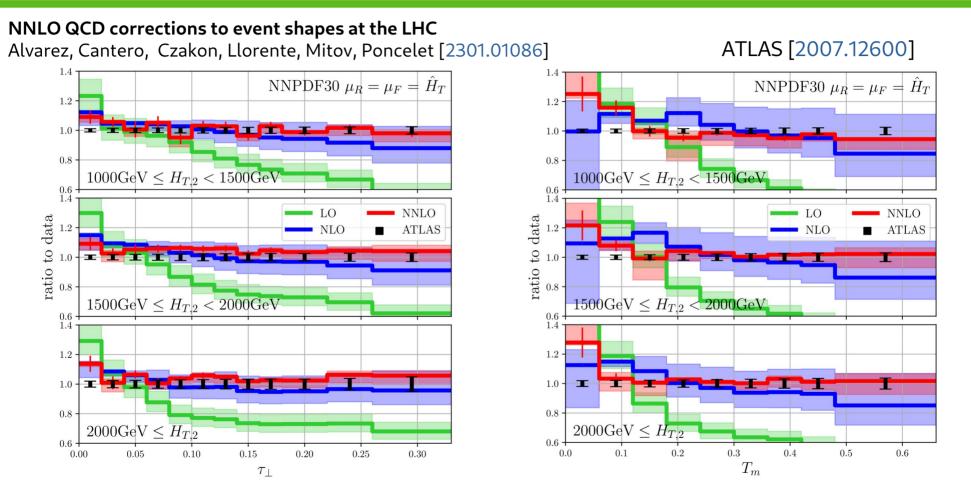


Separation of energy scales: $H_{T,2} = p_{T,1} + p_{T,2}$

Ratio to 2-jet: $R^{i}(\mu_{R}, \mu_{F}, \text{PDF}, \alpha_{S,0}) = \frac{\mathrm{d}\sigma_{3}^{i}(\mu_{R}, \mu_{F}, \text{PDF}, \alpha_{S,0})}{\mathrm{d}\sigma_{2}^{i}(\mu_{R}, \mu_{F}, \text{PDF}, \alpha_{S,0})}$

Here: use jets as input → experimentally advantageous (better calibrated, smaller non-pert.)

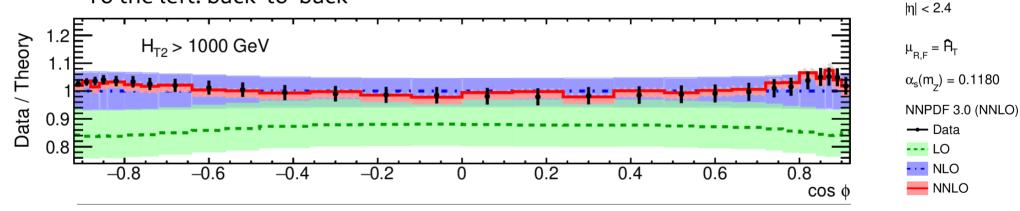
Transverse Thrust @ NNLO QCD



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$$\frac{1}{\sigma_2} \frac{\mathrm{d}\sigma}{\mathrm{d}\cos\Delta\phi} = \frac{1}{\sigma_2} \sum_{ij} \int \frac{\mathrm{d}\sigma \; x_{\perp,i} x_{\perp,j}}{\mathrm{d}x_{\perp,i} \mathrm{d}x_{\perp,j} \mathrm{d}\cos\Delta\phi_{ij}} \delta(\cos\Delta\phi - \cos\Delta\phi_{ij}) \mathrm{d}x_{\perp,i} \mathrm{d}x_{\perp,j} \mathrm{d}\cos\Delta\phi_{ij} \,,$$

- Insensitive to soft radiation through energy weighting $x_{T,i} = E_{T,i} / \sum E_{T,j}$
- Event topology separation:
 - Central plateau contain isotropic events
 - To the right: self-correlations, collinear and in-plane splitting
 - To the left: back-to-back



[ATLAS 2301.09351]

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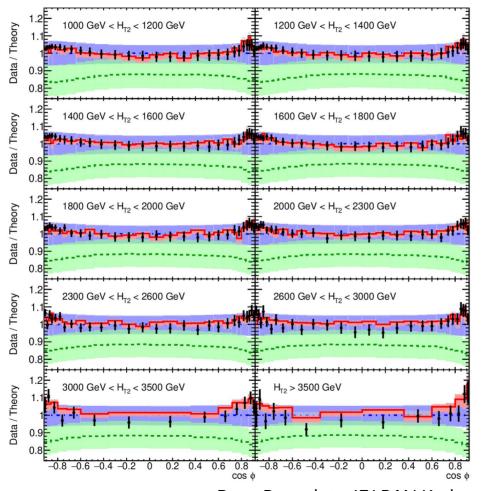
ATLAS

anti- $k_{+}R = 0.4$

 $p_{\tau} > 60 \text{ GeV}$

Particle-level TEEC $\sqrt{s} = 13 \text{ TeV}; 139 \text{ fb}^{-1}$

Double differential TEEC



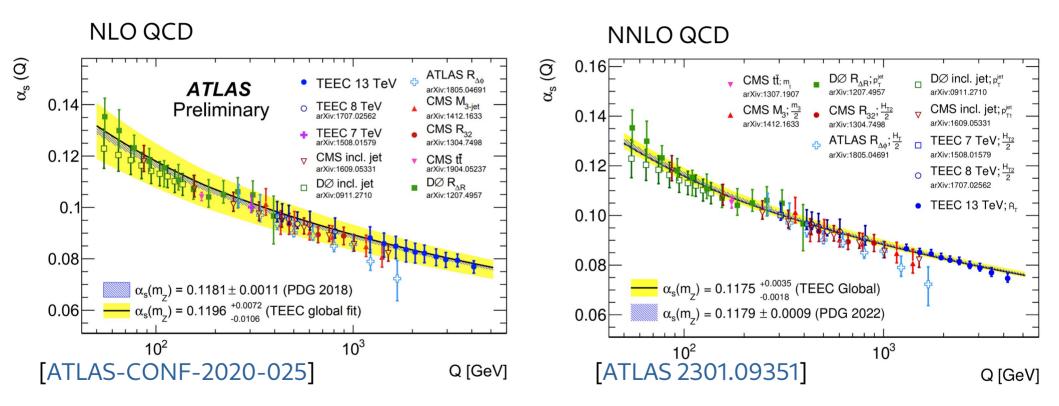
[ATLAS 2301.09351]

ATLAS

Particle-level TEEC √s = 13 TeV; 139 fb⁻¹ anti- $k_{t} R = 0.4$ $p_{_{T}} > 60 \text{ GeV}$ |η| < 2.4 $\mu_{R,F} = \mathbf{\hat{H}}_{T}$ $\alpha_{\rm s}({\rm m_{z}}) = 0.1180$ NNPDF 3.0 (NNLO) - Data --- LO - NLO - NNLO

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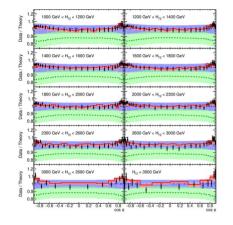
Running of $\alpha_{\mathbf{S}}$



HighTEA

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HighTEA





How to make this more efficient/environment-friendly/ accessible/faster?

HighTEA: **High energy Theory Event Analyser** [2304.05993]

Michał Czakon,^a Zahari Kassabov,^b Alexander Mitov,^c Rene Poncelet,^c Andrei Popescu^c

^a Institut für Theoretische Teilchenphysik und Kosmologie, RWTH Aachen University, D-52056 Aachen, Germany

^bDAMTP, University of Cambridge, Wilberforce Road, Cambridge, CB3 0WA, United Kingdom ^cCavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom *E-mail:* mczakon@physik.rwth-aachen.de, zk261@cam.ac.uk, adm74@cam.ac.uk, poncelet@hep.phy.cam.ac.uk, andrei.popescu@cantab.net

https://www.precision.hep.phy.cam.ac.uk/hightea

high tead for your freshly brewed analysis

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- Database of precomputed "Theory Events"
 - Equivalent to a full fledged computation
 - ➤ Currently this means partonic fixed order events
 - Extensions to included showered/resummed/hadronized events is feasible
 - → (Partially) Unweighting to increase efficiency
- Analysis of the data through an user interface
 - ✤ Easy-to-use
 - → Fast

- Observables from basic 4-momenta
- Free specification of bins
- Flexible: Renormalization/Factorization Scale variation
 - PDF (member) variation
 - Specify phase space cuts

Not so new idea: LHE [Alwall et al '06], Ntuple [BlackHat '08'13],

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Factorizations

Factorizing renormalization and factorization scale dependence:

$$w_{s}^{i,j} = w_{\text{PDF}}(\mu_{F}, x_{1}, x_{2}) w_{\alpha_{s}}(\mu_{R}) \left(\sum_{i,j} c_{i,j} \ln(\mu_{R}^{2})^{i} \ln(\mu_{F}^{2})^{j} \right)$$

PDF dependence:

$$w_{\text{PDF}}(\mu, x_1, x_2) = \sum_{ab \in \text{channel}} f_a(x_1, \mu) f_b(x_2, \mu)$$

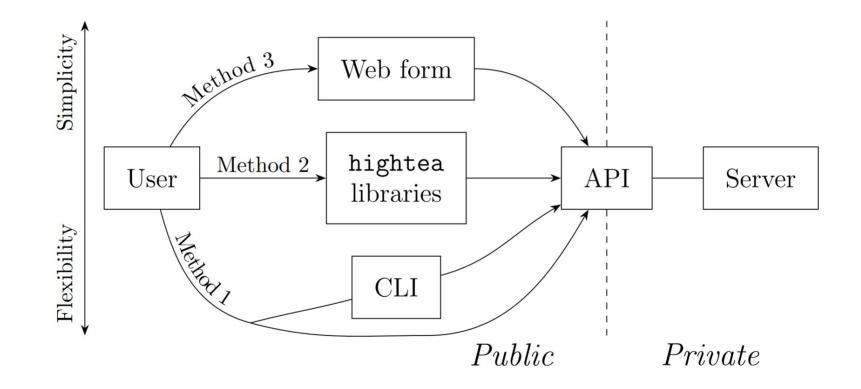
 α_s dependence:

 $w_{\alpha_s}(\mu) = (\alpha_s(\mu))^m$

Allows full control over scales and PDF

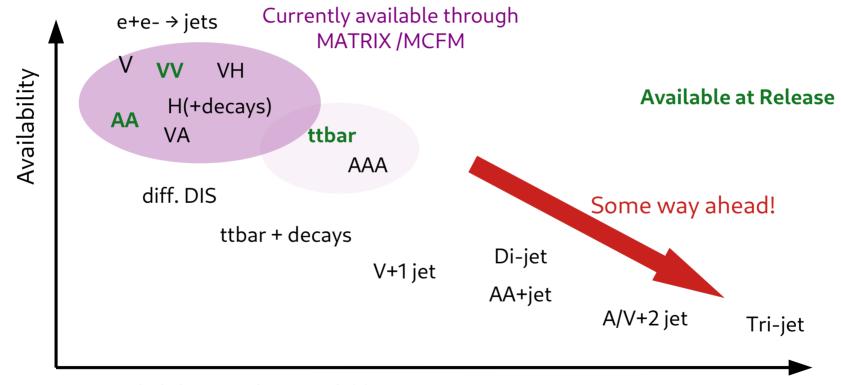
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HighTEA interface



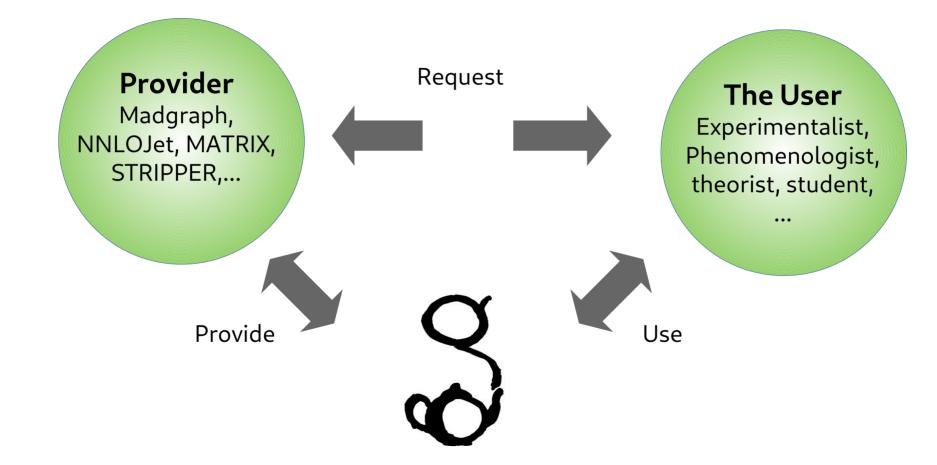
Available Processes

Processes currently implemented in our STRIPPER framework through NNLO QCD



Complexity

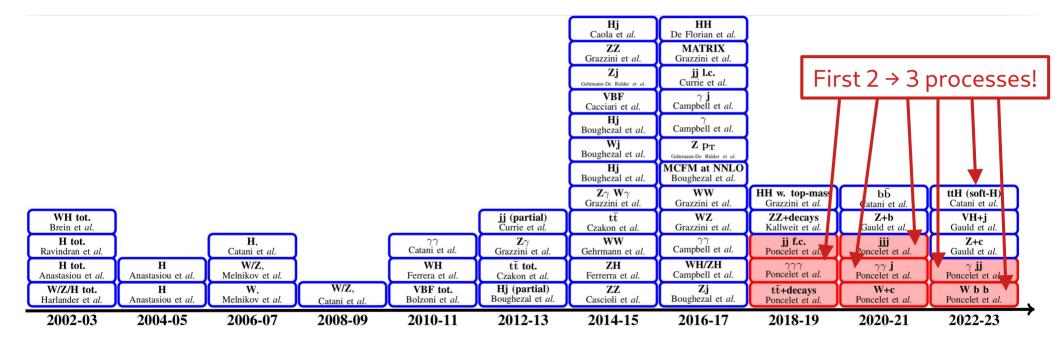
The Vision



Summary & Outlook

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The NNLO QCD revolution



- Subtraction at NNLO QCD gains maturity, challenges remain...
 - Efficiency!
 - Still difficult to run codes!
 - HighTEA possible solution?!
- Two-loop matrix elements for high multiplicity are the single most significant bottleneck for NNLO QCD calculations
 - 2 to 3 massless ME completed in full colour (~10 years of work of ~5 research groups)
 - 1 mass MEs next challenge...
- NNLO QCD is a staple for SM precision phenomenology
 - Challenge: matching to parton-shower!

Backup

18.12.23 Göttingen

Phase space cut and differential observable introduce *mis-binning* : mismatch between kinematics in subtraction terms → leads to increased variance of the integrand → slow Monte Carlo convergence

New phase space parametrization [Czakon'19]:

Minimization of # of different subtraction kinematics in each sector

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Mapping from n+2 to n particle phase space:

Requirements:

$$\{P, r_j, u_k\} \to \left\{\tilde{P}, \tilde{r}_j\right\}$$

- Keep direction of reference r fixed
- Invertible for fixed u_i : $\{\tilde{P}, \tilde{r}_j, u_k\} \rightarrow \{P, r_j, u_k\}$ Preserve Born invariant mass: $q^2 = \tilde{q}^2, \quad \tilde{q} = \tilde{P} \sum_{i=1}^{n_{fr}} \tilde{r}_j$ Main steps:
- Generate Born configuration
- Generate unresolved partons u_i
- Rescale reference momentum $r = x\tilde{r}$
- Boost non-reference momenta of the Born configuration

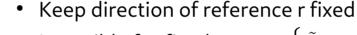
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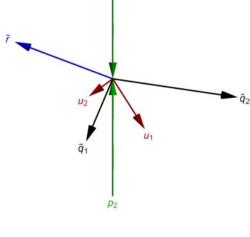
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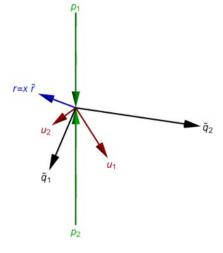
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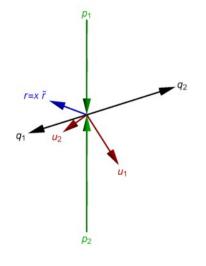
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