Precision Measurements - Theory

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Current issues

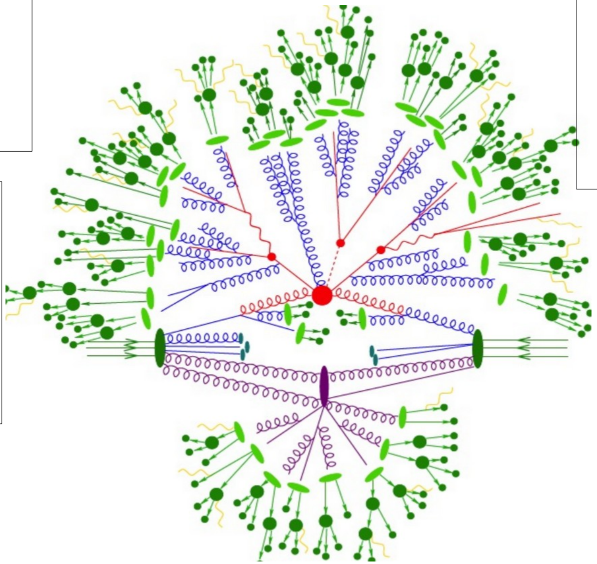
NNLO + PS
→ generality
→ accuracy

Theory uncertainties
→ fixed-order
→ resummation
→ PDFs (aN3LO/flavour schemes)

Mixed EW x QCD corrections
→ amplitudes
→ subtraction

Flavoured jets
→ flavoured algorithms
→ experimental implementation

FO subtraction schemes at NNLO
→ generality & efficiency
→ numerical integration



[Credit: SHERPA]

Toponium/top-pair threshold
→ bound state
→ resummation

Multi-loop amplitudes
→ Methods
→ Automation

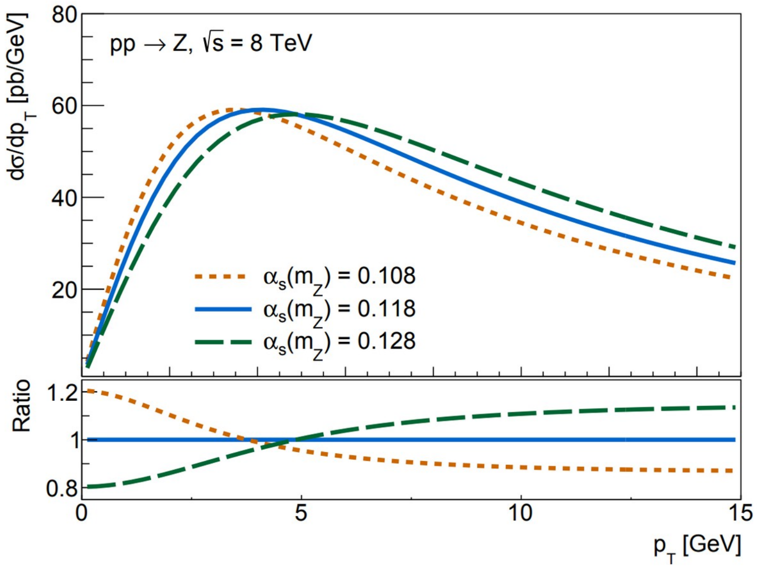
...

Theory uncertainties

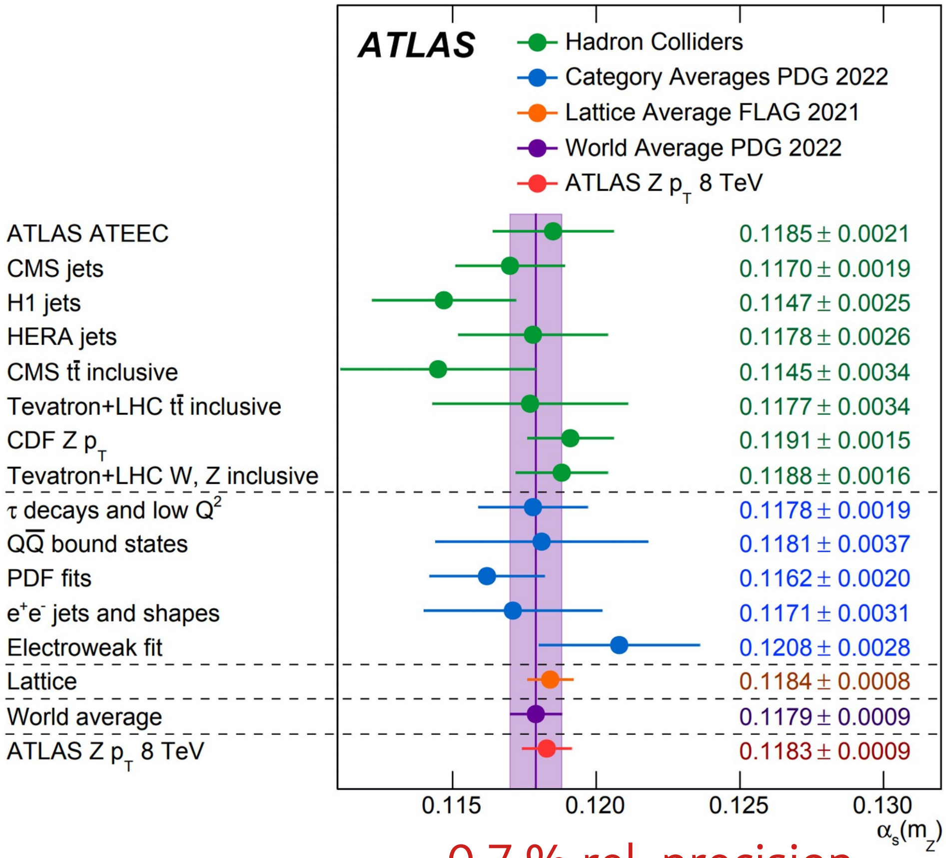
Precision example: strong coupling from pT(Z)

[ATLAS 2309.12986]

Sensitivity of Z-boson's recoil to the strong coupling constant:



→ at low pT resummation regime!
→ theory uncertainty?



~0.7 % rel. precision

Theory uncertainties in Higgs production

[LHCH(XS)WG YR4' 16]

Input parameters

$\sqrt{S}$	13 TeV
m_h	125 GeV
PDF	PDF4LHC15_nnlo_100
$\alpha_s(m_Z)$	0.118
$m_t(m_t)$	162.7 GeV ($\overline{\text{MS}}$)
$m_b(m_b)$	4.18 GeV ($\overline{\text{MS}}$)
$m_c(3GeV)$	0.986 GeV ($\overline{\text{MS}}$)
$\mu = \mu_R = \mu_F$	62.5 GeV ($= m_H/2$)

N4LO approximation
[Das, Moch, Vogt '20]

aN3LO PDFs
[MSHT'22]
[NNPDF'24]

Exact top-mass dependence through NNLO QCD
[Czakon, Harlander, Klappert, Niggetiedt'21]

δ(scale)	δ(trunc)	δ(PDF-TH)	δ(EW)	$\delta(t,b,c)$	$\delta(1/m_t)$
$^{+0.10\text{ pb}}_{-1.15\text{ pb}}$	±0.18 pb	±0.56 pb	±0.49 pb	±0.40 pb	±0.49 pb
$^{+0.21\%}_{-2.37\%}$	$\pm0.37\%$	$\pm1.16\%$	$\pm1\%$	$\pm0.83\%$	$\pm1\%$

N3LO HEFT
[Mistlberger'18]

Improved QCD-EW predictions
[Bonetti, Melnikov, Trancredi'18] [Anastasiou et al '19]
[Bonetti et al. '20][Bechetti et al. '21] [Bonetti, Panzer, Trancredi '22]

Bottom-top-interference
[Czakon, Eschment, Niggetiedt, Poncelet, Schellenberger `23,`24]

Uncertainties in precision phenomenology

Experiments are getting more precise → theory uncertainties matter!

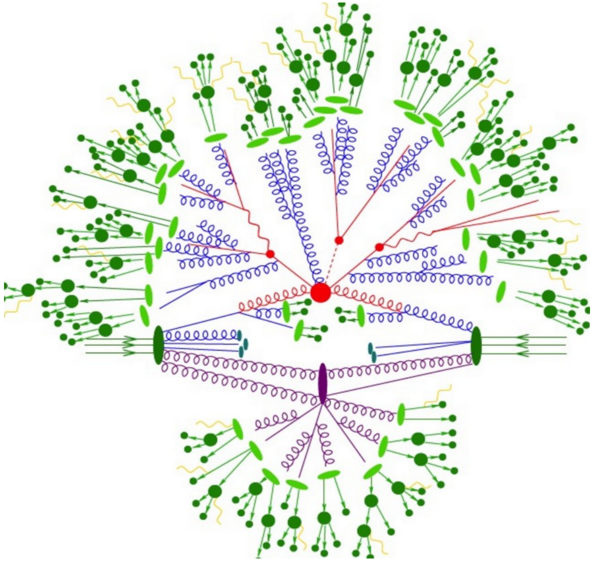
Sources of theory uncertainties:

- parametric (values of coupling parameters etc.)
→ variation of parameters within their uncertainties

- parton distribution functions (PDFs)
→ different error propagation methods (fit parameter, replicas,...)

- non-perturbative parameters in Monte Carlo simulations.
→ needs data constraints by definition. Problematic if dominant effect...

- missing higher orders in fixed-order and resummed predictions (MHOU)
→ tricky because we are trying to estimate the unknown….



[Credit: SHERPA]

Missing higher orders

Notation from: [Tackmann 2411.18606]
Beyond Scale Variations: Perturbative Theory Uncertainties from Nuisance Parameters

Generic perturbative expansion:

$$f(\alpha) = f_0 + f_1\alpha + f_2\alpha^2 + f_3\alpha^3 + \dots$$

f_i : the coefficient of the series, potentially unknown

We can compute the truncated series: $\hat{f}_i$: the true value, i.e. a value we actually computed

$$f^{\mathrm{LO}}(\alpha) = \hat{f}_0 \qquad f^{\mathrm{NLO}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha \qquad f^{\mathrm{NNLO}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + \hat{f}_2\alpha^2$$

The missing terms are the source of uncertainty.
(assume convergence → the first missing is the dominant one)

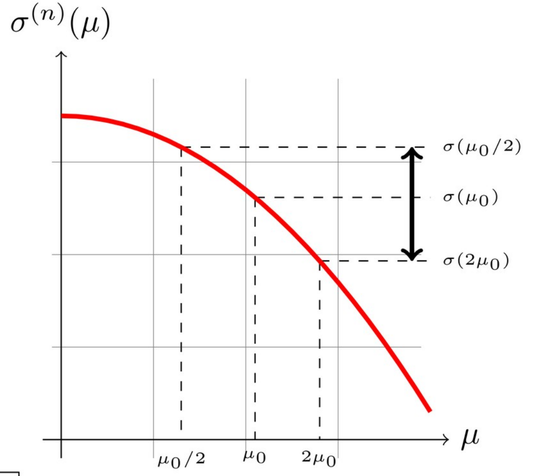
$$f^{\mathrm{LO+1}}(\alpha) = \hat{f}_0 + f_1\alpha \quad f^{\mathrm{NLO+1}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + f_2\alpha^2 \quad f^{\mathrm{NNLO+1}}(\alpha) = \hat{f}_0 + \hat{f}_1\alpha + \hat{f}_2\alpha^2 + f_3\alpha^3$$

Challenge: how to estimate f_1, f_2, f_3, … without computing them?

Theory uncertainties from scale variations

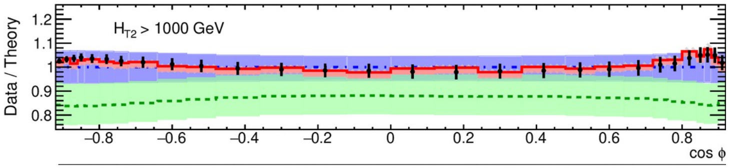
Lets focus on QCD as an example: $\alpha = \alpha_s(\mu_0)$

$$\mathrm{d}\sigma = \mathrm{d}\sigma^{(0)} + \alpha_s \mathrm{d}\sigma^{(1)} + \alpha_s^2 \mathrm{d}\sigma^{(2)} + \ldots \xrightarrow{\text{RGE}} \mu \frac{\mathrm{d}\sigma^{(n)}}{\mathrm{d}\mu} = \mathcal{O}\left(^{(n_0+n+1)}\right)$$

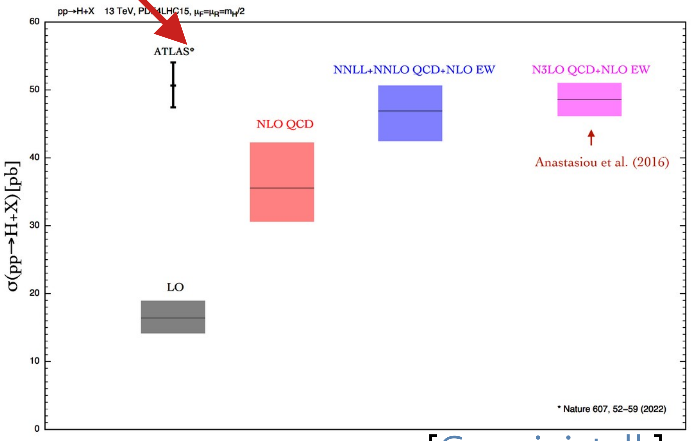


Of same order as the next dominant term
→ exploiting this to estimate size of $\mathrm{d}\sigma^{(n+1)}$

Sometimes it does works … sometimes not



[ATLAS 2301.09351]



[Grazzini, talk]

Short comings of scale variations

- not always reliable … however in most cases issues are understood/expected:
  new channels, phase space constraints, etc. → often we can design workarounds
- however, some issues are more fundamental:
  → how to choose the central scale? → not a physical parameter, no ‘true’ value
  (Principle of fasted apparent convergence, principle of minimal sensitivity,…)
  → how to propagate the estimated uncertainty, no statistical interpretation!
  → what about correlations? Based on ‘fixed form’ of the lower orders and RGE.

(At the moment) two alternative approaches under investigation:

“Bayesian”

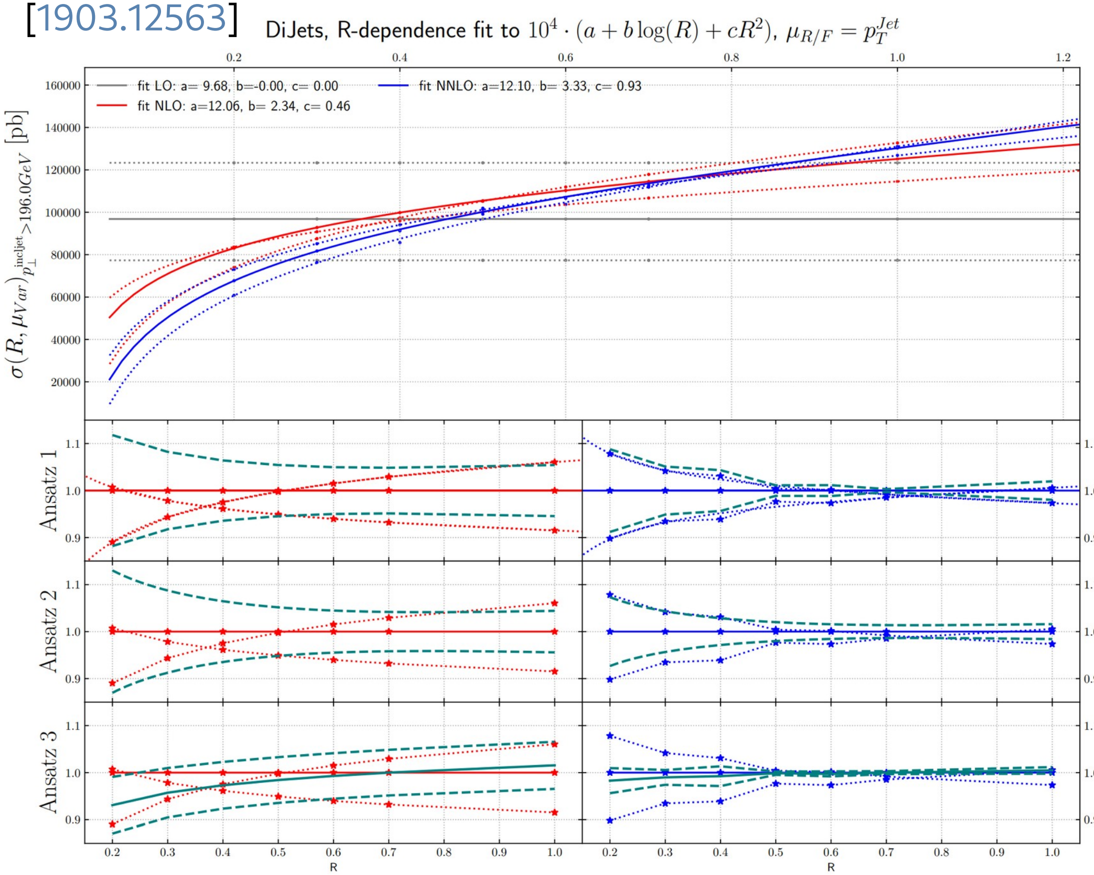
[Cacciari,Houdeau 1105.5152]
[Bonvini 2006.16293]
[Duhr, Huss, Mazeliauskas, Szafron 2106.04585]

“Theory Nuisance Parameter”

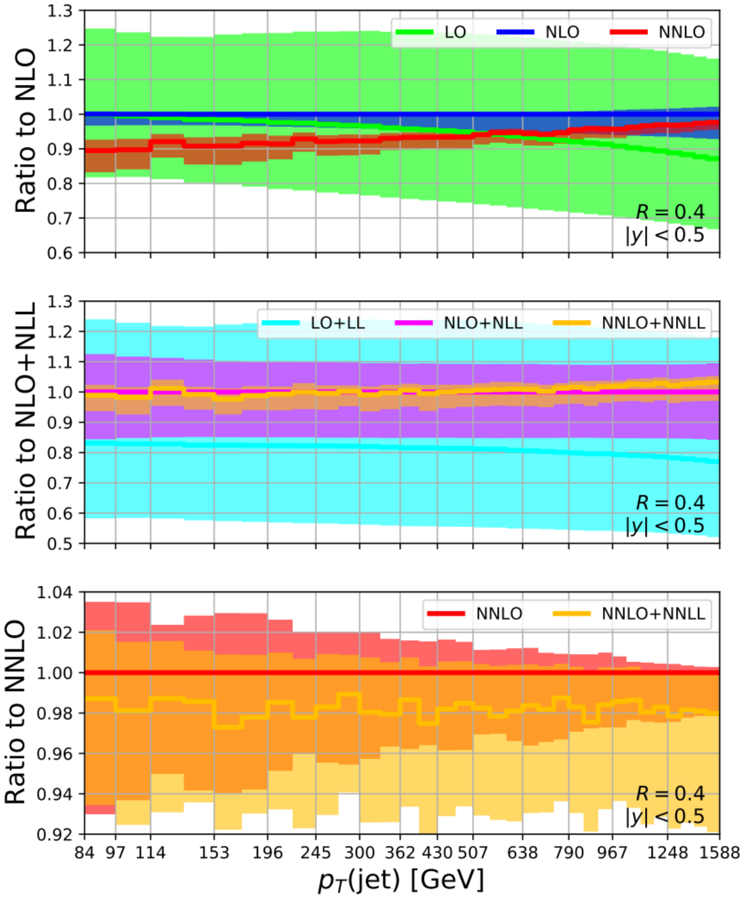
[Tackmann 2411.18606]
→ W mass extraction: [CMS 2412.13872]
[Cal,Lim, Scott,Tackmann Waalewijn 2408.13301]
[Lim, Poncelet, 2412.14910]

Example: uncertainties in jet cross sections

[1903.12563]



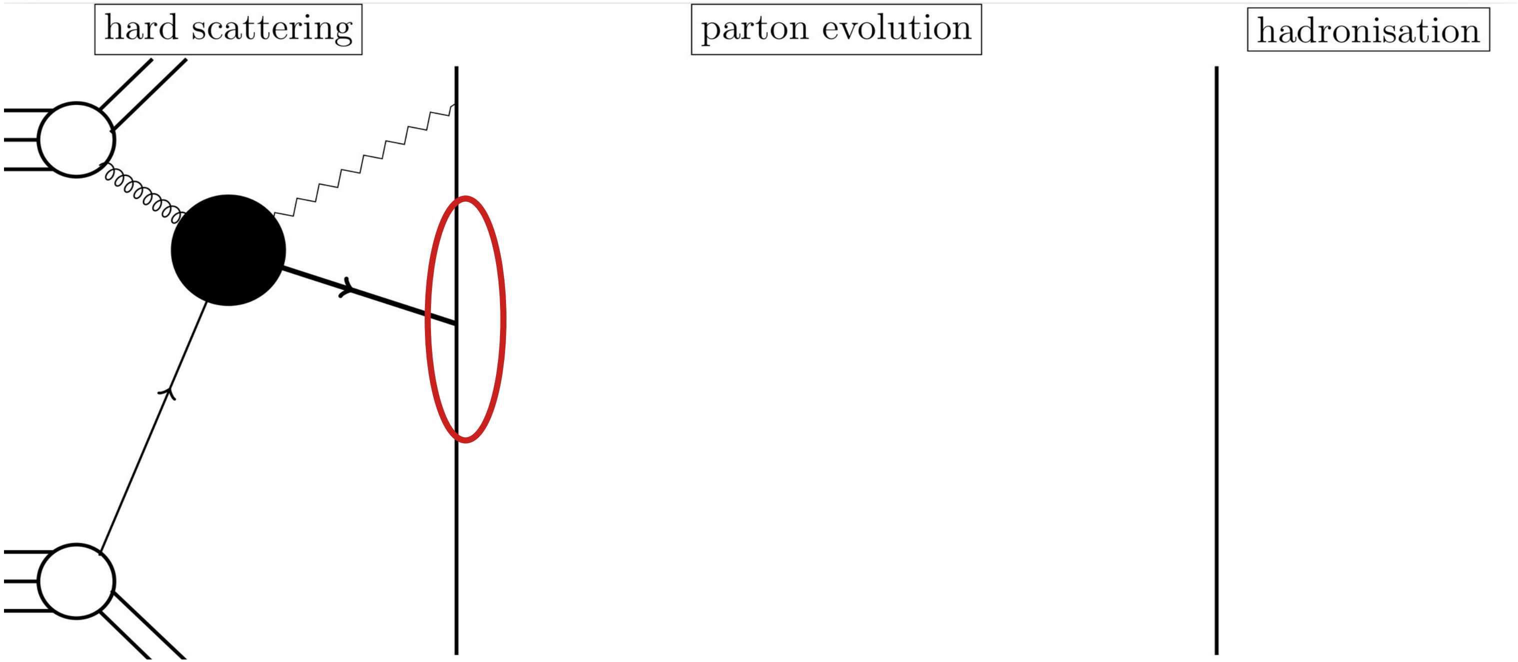
[2503.21866]



Flavoured jets

Flavoured jets

jet that initiated from a "hard scatter” product of specific flavour:
bottom, charm , "quark/gluon"



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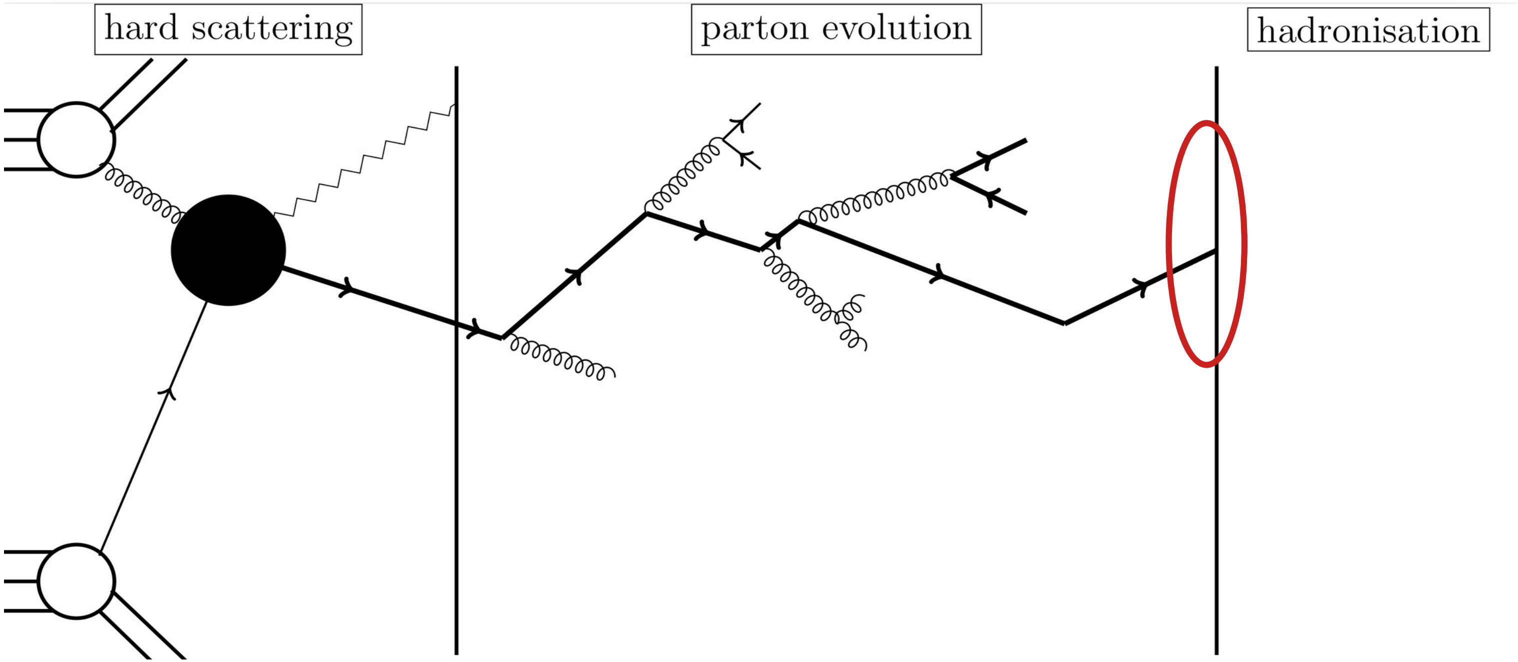

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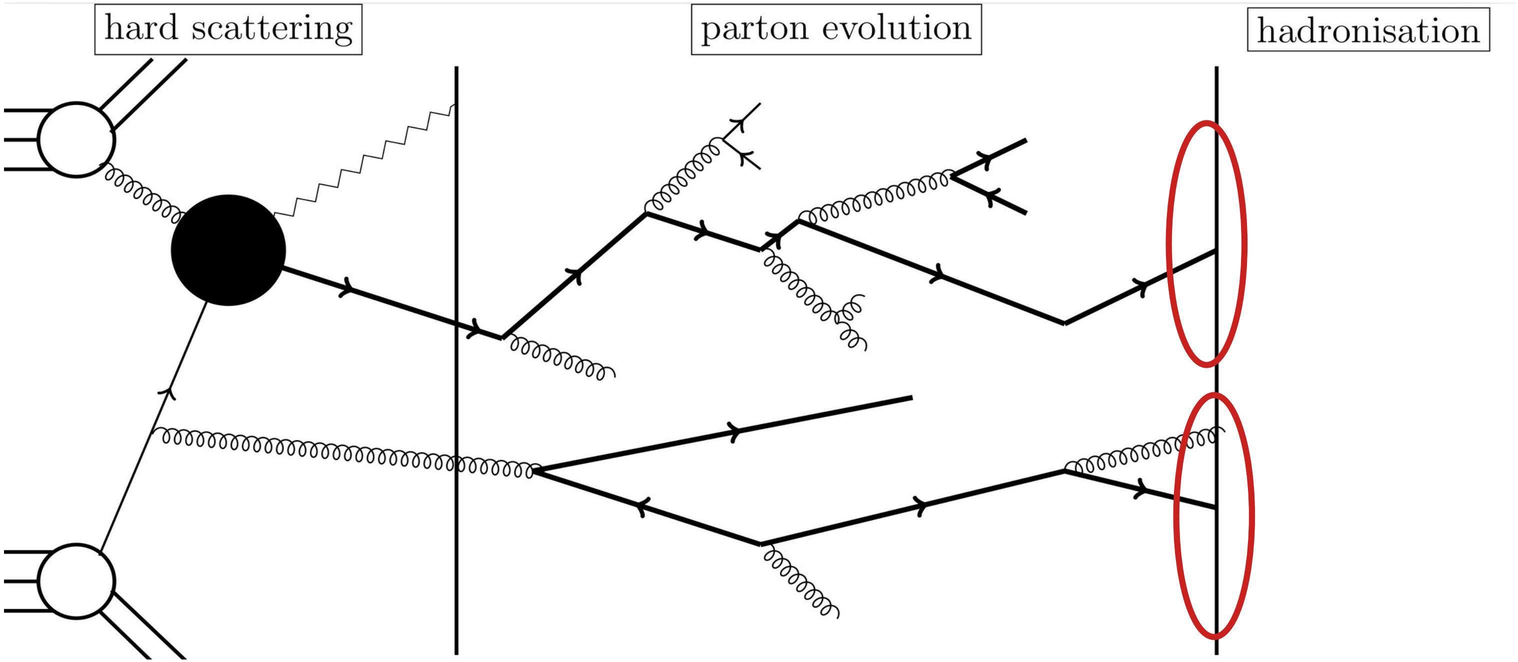

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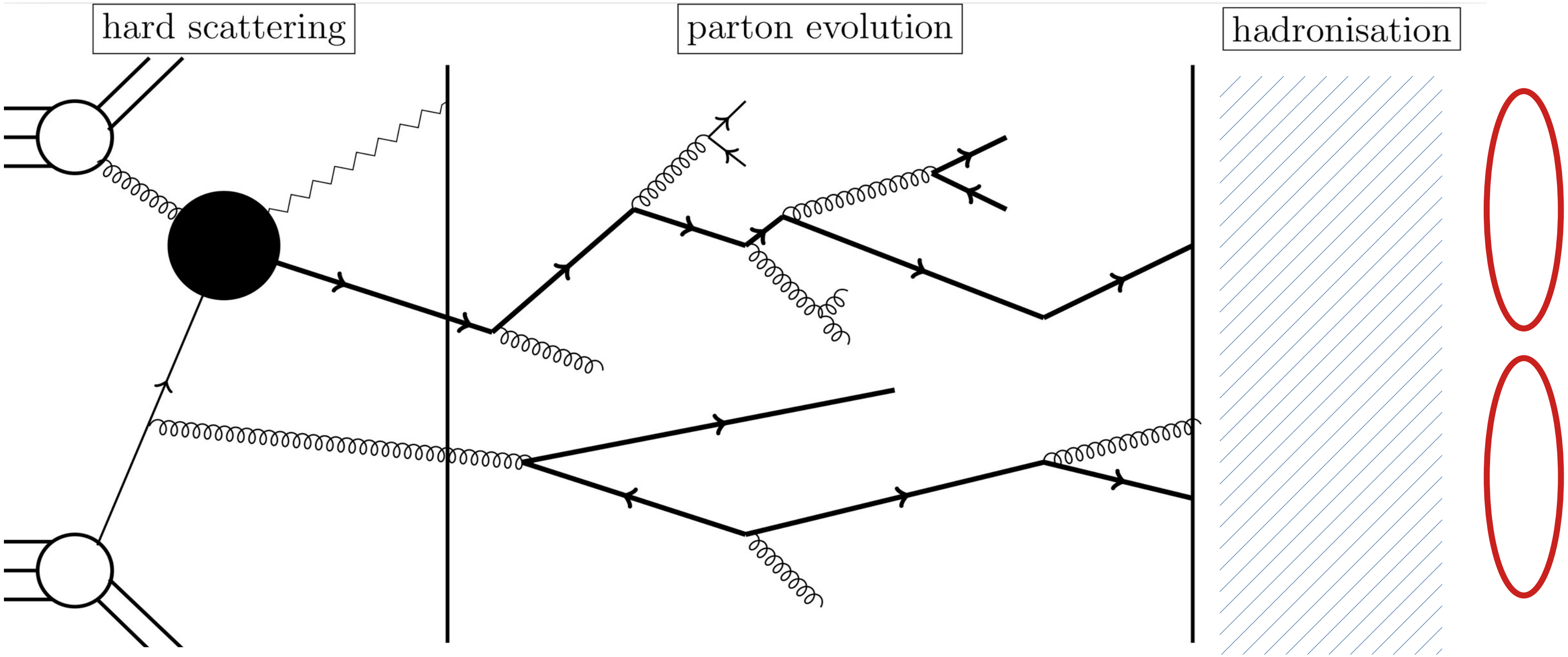
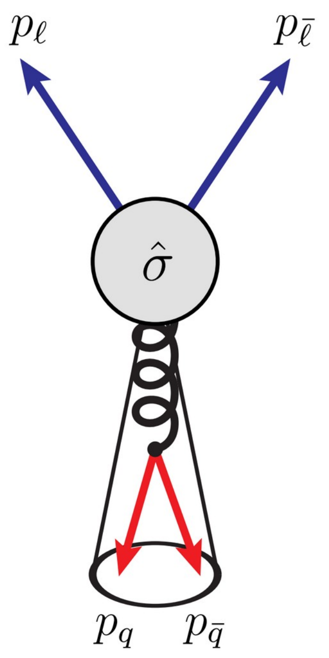


Infrared safety issues with flavoured jets I



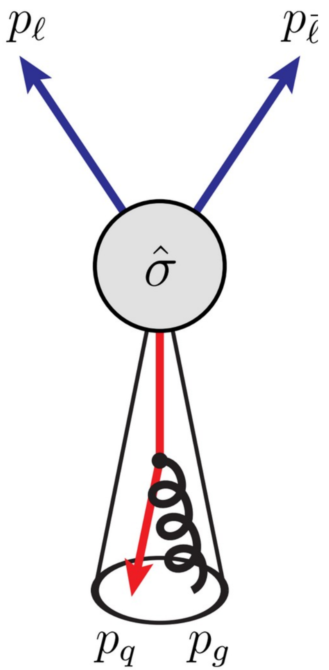
Picture from
[Gauld et al. 2302.12844]

- IRC unsafe due to g→quark-anti-quark splitting
  - Quarks massless: cross-section not defined
  - Quarks massive: logarithmic sensitivity to quark mass
- Can resolved by proper flavour recombination schemes:

scheme \ jet contents	b	$b+\bar{b}$	$b+b$	
"any flavour"	b	b	b	simplest experimentally (but collinear unsafe for $m_b \to 0$)
net flavour	b	g	$2b$	theoretically "ideal" definition; but not robust wrt B–Bbar oscillations
flavour modulo 2	b	g	g	theoretically OK; robust wrt B–Bbar oscillations

[Salam]

Infrared safety issues with flavoured jets II

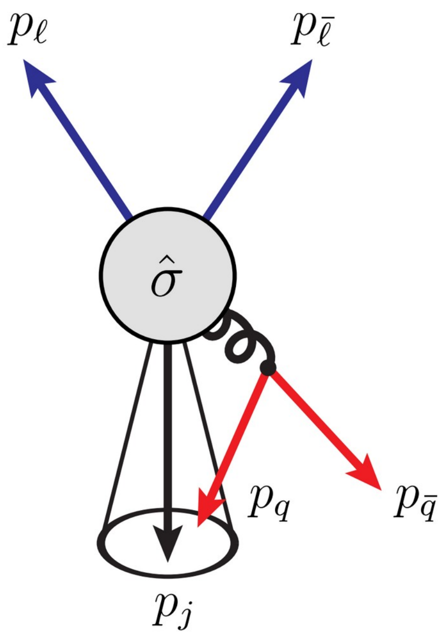


Picture from
[Gauld et al. 2302.12844]

- Collinear unsafe if pT requirement on the quark is present
- Not implementable in pQCD with massless quarks
  → proper treatment needs fragmentation functions
  → NNLO QCD example:

B-hadron production in NNLO QCD: application to LHC ttbar events with leptonic decays, Czakon, Generet, Mitov and Poncelet, 2102.08267

Infrared safety issues with flavoured jets III



Picture from
[Gauld et al. 2302.12844]

- Starting at NNLO QCD:
  → Soft singularity from quark pairs
  - Massless quarks → cross section not defined
  - Massive quarks → logarithmic IRC sensitivity $\ln\left(\frac{m}{p_T}\right)$
- Needs modified jet algorithms!

New proposals for flavour-safe anti-kT jets

- Flavour with Soft-drop

  Practical Jet Flavour Through NNLO
  Caletti, Larkoski, Marzani, Reichelt 2205.01109

- Flavour anti-kT

  Infrared-safe flavoured anti-kT jets,
  Czakon, Mitov, Poncelet 2205.11879

- Fragmentation approach

  A Fragmentation Approach to Jet Flavor
  Caletti, Larkoski, Marzani, Reichelt 2205.01117

  B-hadron production in NNLO QCD: application to LHC ttbar events with leptonic decays,
  Czakon, Generet, Mitov and Poncelet, 2102.08267

- Flavour dressing → standard anti-kT + flavour assignment

  QCD-aware partonic jet clustering for truth-jet flavour labelling
  Buckley, Pollard 1507.00508

  A dress of flavour to suit any jet
  Gauld, Huss, Stagnitto 2208.11138

- Interleaved flavour neutralisation

  Flavoured jets with exact anti-kT kinematics and tests of infrared and collinear safety
  Caola, Grabarczyk, Hutt, Salam, Scyboz, Thaler 2306.07314

- TBC...

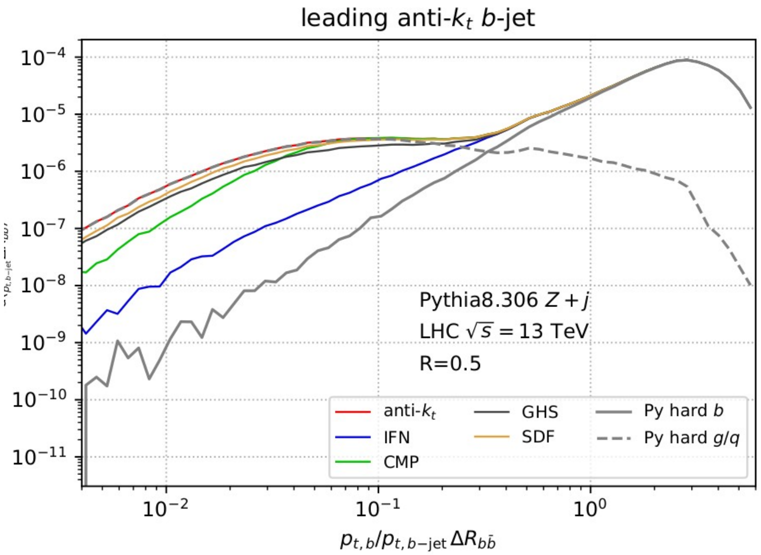
Outcome LH23

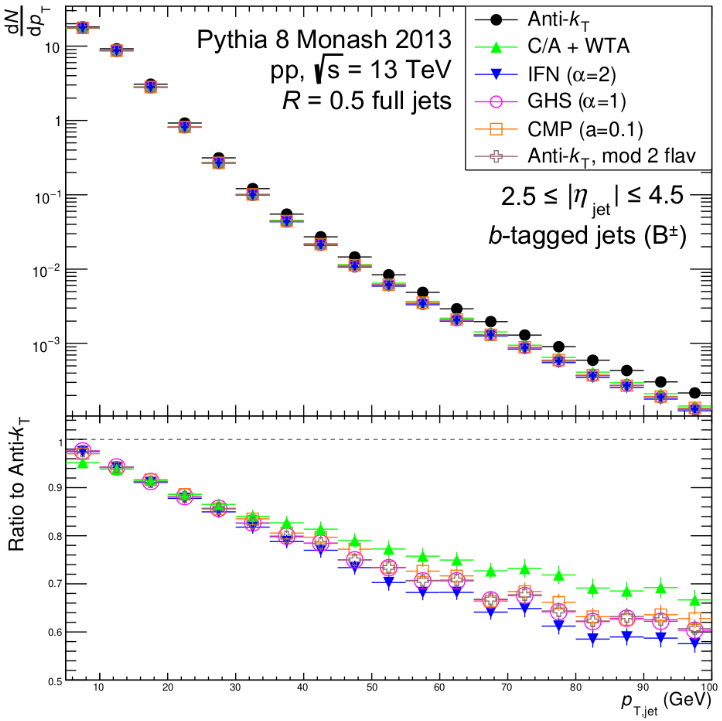
Today on the arxiv

Flavoured jet algorithms: a comparative study

Arnd Behring,[1] Simone Caletti,[2] Francesco Giuli,[3] Radosław Grabarczyk,[4,5] Andreas Hinzmann,[6] Alexander Huss,[7] Joey Huston,[8] Ezra D. Lesser,[7] Simone Marzani,[9] Davide Napoletano,[10] Rene Poncelet,[11] Daniel Reichelt,[7,12] Alberto Rescia,[9] Gavin P. Salam,[5,14] Ludovic Scyboz,[15] Federico Sforza,[9] Andrzej Siódmok,[7,16] Giovanni Stagnitto,[10] James Whitehead,[16] Ruide Xu[17]

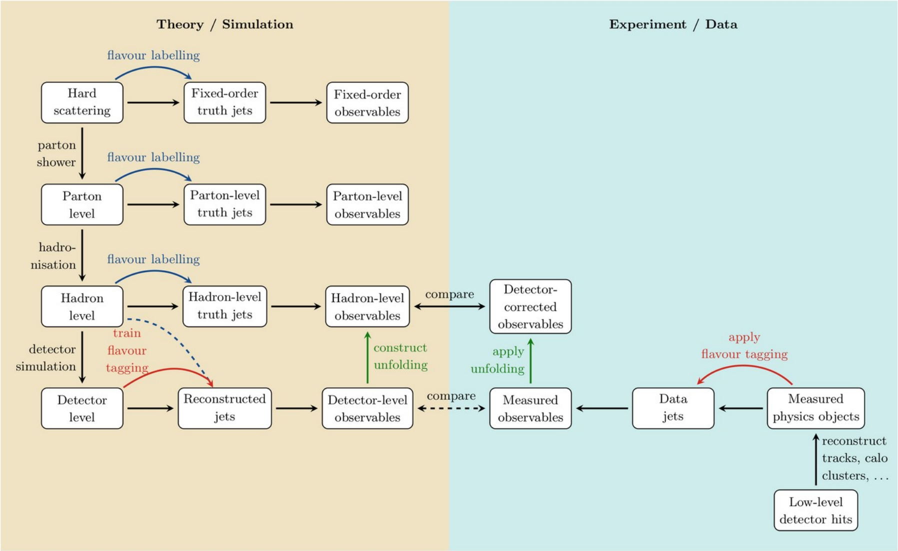
Many analyses from theory and experiment groups → improved understanding on all sides

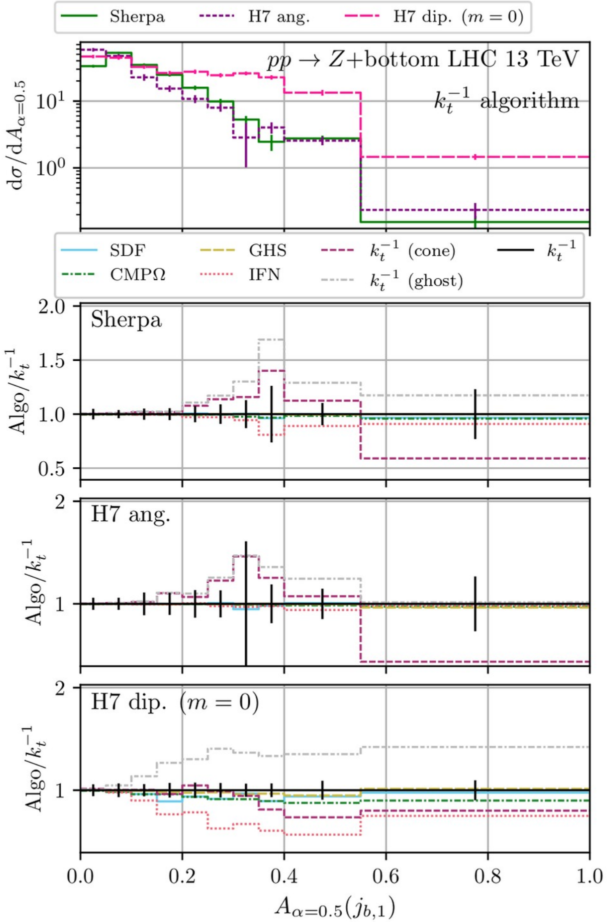




Open Questions

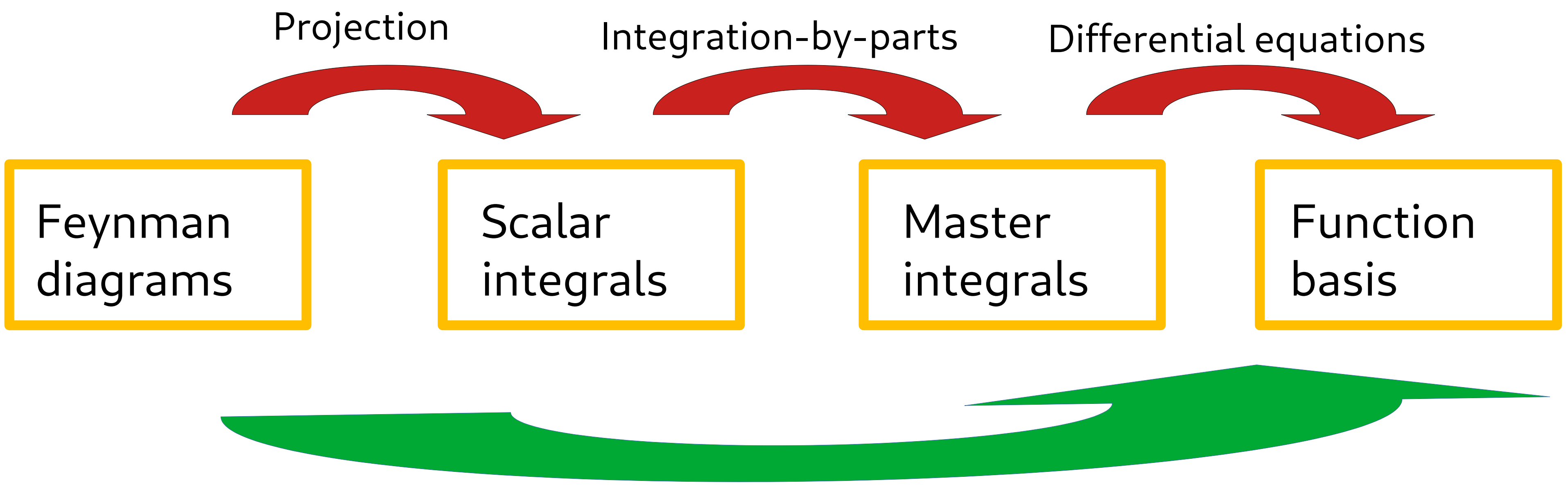
→ impact of hadronisation?
→ impact on jet substructure?
→ how to incorporate in experiment?
→ revisit the truth level labels in the training of ML taggers?
→ can we get an experimental handle on $g \to f\bar{f}$?





Amplitudes

Typical multi-loop calculation work-flow



Finite Field methodology to circumvent
excessively large intermediate expressions

Integration-By-Parts reduction

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

→ 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

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

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

Master integrals

Differential Equations: $\mathrm{d}\vec{\mathrm{MI}} = \mathrm{d}A(\{p\},\epsilon)\vec{\mathrm{MI}}$

Canonical basis: $\mathrm{d}\vec{\mathrm{MI}} = \epsilon\mathrm{d}\tilde{A}(\{p\})\vec{\mathrm{MI}}$

[Remiddi, 97]
[Gehrmann, Remiddi, 99]
[Henn, 13]

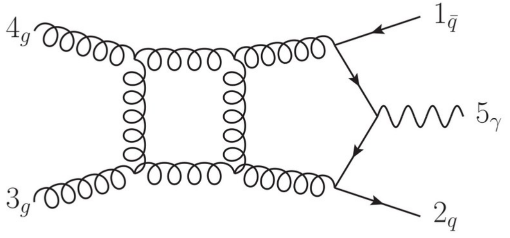
Simple iterative solution

$$\mathrm{MI}_i = \sum_w \epsilon^w \tilde{\mathrm{MI}}_i^w \quad \text{with} \quad \tilde{\mathrm{MI}}_i^w = \sum_j c_{i,j} m_j$$

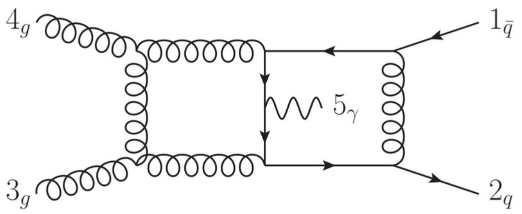
Chen-iterated integrals
"Pentagon"-functions

[Chicherin, Sotnikov, 20]
[Chicherin, Sotnikov, Zoia, 21]

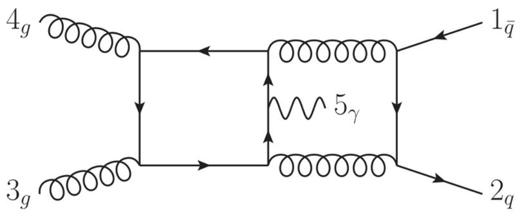
Reconstruction of Amplitudes



$A^{(2),N_c^2}_{34;q}$, $A^{(2),N_c}_{\delta;q}$



$A^{(2),1}_{34;q}$, $A^{(2),N_c}_{\delta;q}$, $A^{(2),1/N_c}_{\delta;q}$



$A^{(2),N_c}_{34;l}$, $A^{(2),1/N_c}_{34;l}$, $A^{(2),1/N_c^2}_{\delta;l}$

[Badger et al '23]

Many possible optimizations

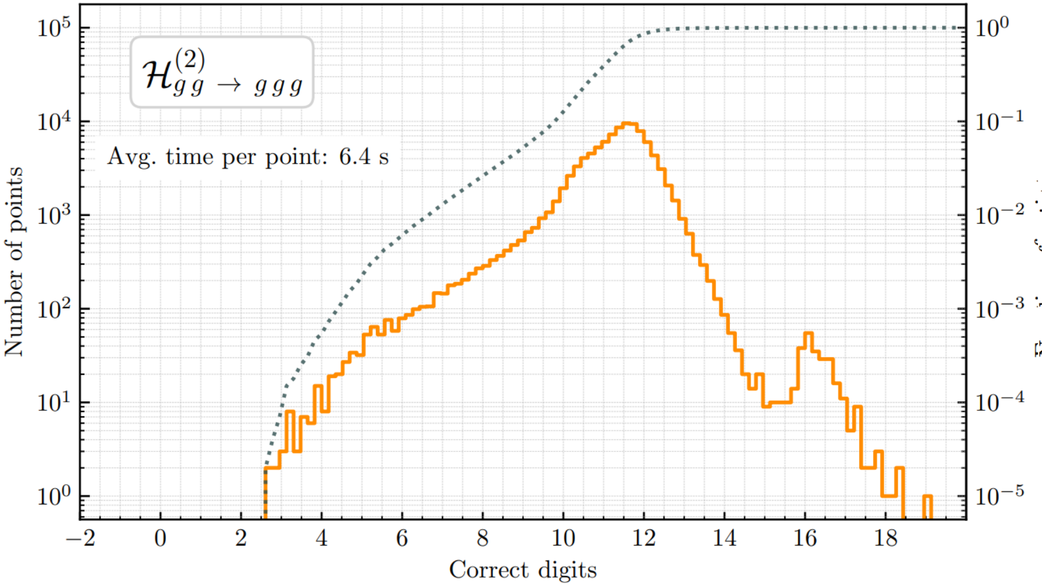
- Syzygy's to simplify IBPs
- Exploitation of Q-linear relations
- Denominator Ansaetze
- On-the-fly partial fractioning
- ...

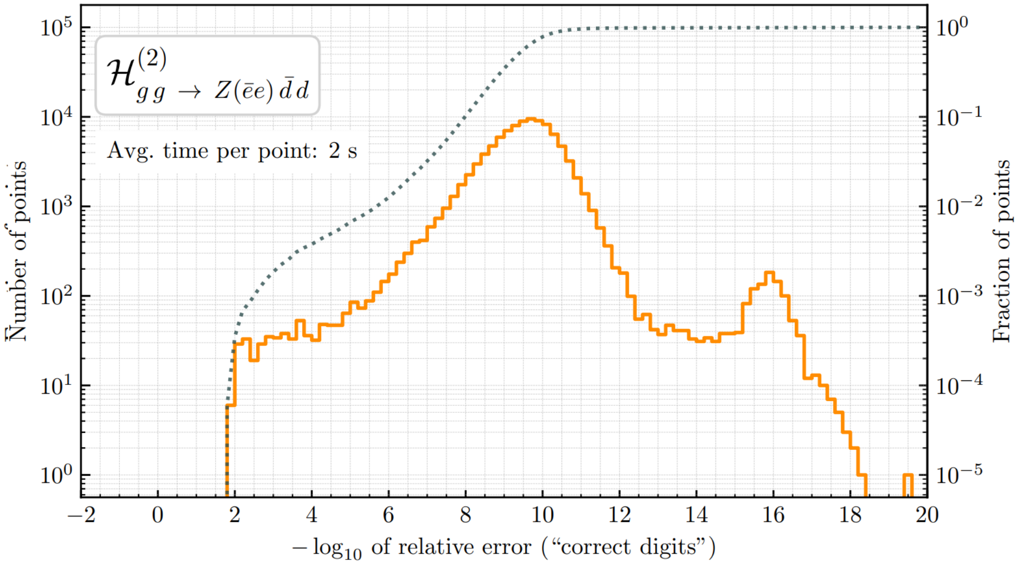
amplitude	helicity	original	stage 1	stage 2	stage 3	stage 4
$A^{(2),1}_{34;q}$	$-++-+$	94/91	74/71	74/0	22/18	22/0
$A^{(2),1}_{34;q}$	$-+-++$	93/89	90/86	90/0	24/14	18/0
$A^{(2),1/N_c^2}_{34;q}$	$-++-+$	90/88	73/71	73/0	23/18	22/0
$A^{(2),1/N_c^2}_{34;q}$	$-+-++$	90/86	86/82	86/0	24/14	19/0
$A^{(2),1/N_c}_{34;l}$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

Reduction of complexity

Numerical evaluation of two-loop matrix elements

[De Laurentis, Ita, Sotnikov’23][De Laurentis, Ita, Page, Sotnikov’25]





Efficient function basis representation power the speed.

If too expensive → numerical interpolation grids (used a lot for 2D problems)?

Methods for high dimensions?

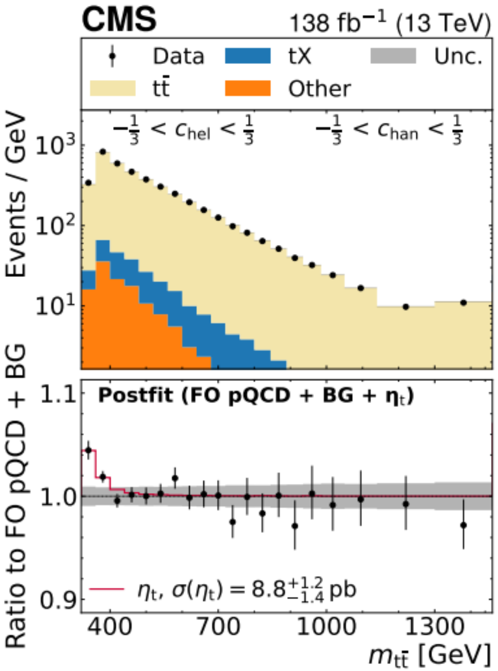
Topics for amplitude discussions

- Geometry, elliptic functions, Calabi-Yau, ...
- Dimensional regularization and gamma5
- Automation @ two-loops
- Standardisation of interfaces
- Efficiency:
  - ML
  - **Interpolation**
  - partial fractioning
  - singularities

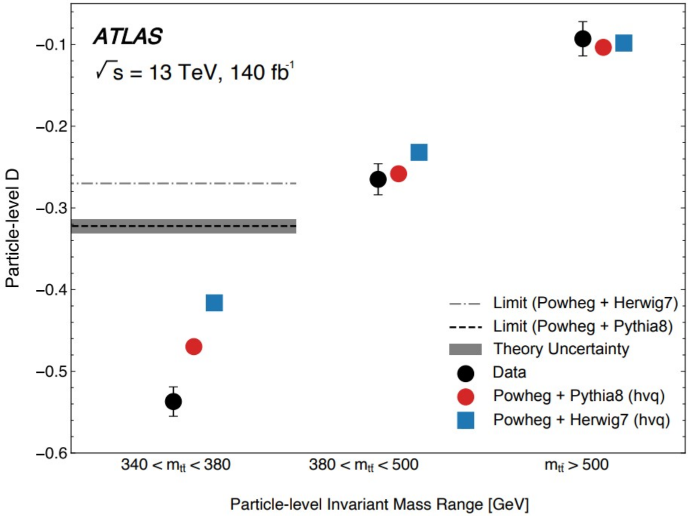
Toponium / top-pair threshold

Surprises at the threshold

[CMS'25] Toponium

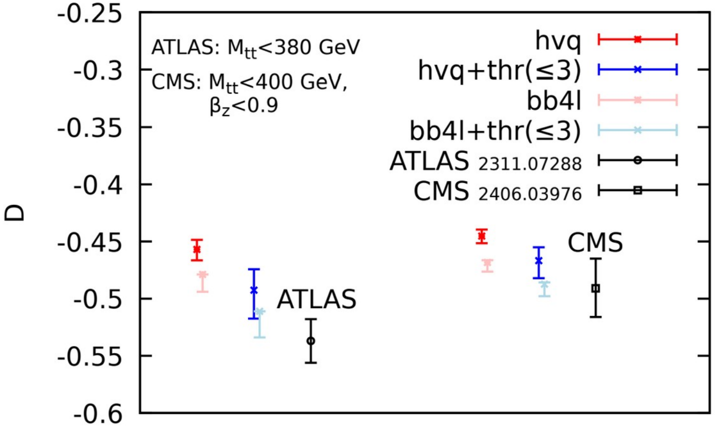


[ATLAS'23] Entanglement



Threshold QCD enhancements

[Nason,Re,Rottoli'25]



Sounds like super topic for a discussion :)

Numerical integration and non-positive integrands or negatively weighted events

The problem

- Numerical integration of highly dimensional integrands → Monte Carlo Sampling

Integral

$$I = \int_{\mathbf{x}\in\Omega} \mathrm{d}\mathbf{x} f(\mathbf{x})$$

MC estimate

$$\hat{I} = \frac{1}{N}\sum_{i=1}^{N} f(\mathbf{x}_i) \, ,$$

MC error estimate

$$\delta\hat{I} = \sqrt{\frac{1}{N-1}\left(\frac{1}{N}\sum_{i=1}^{N} f^2(\mathbf{x}_i) - \hat{I}^2\right)}$$

- Variance reduction techniques improve performance, mapping $\mathbf{H} : \Omega \to \Omega, \mathbf{x} \mapsto \mathbf{H}(\mathbf{x})$

$$I = \int_{\mathbf{H}(\mathbf{x})\in\Omega} \mathrm{d}\mathbf{H} \frac{f(\mathbf{x})}{h(\mathbf{x})}$$

$$h(\mathbf{x}) = \left|\det\left(\frac{\partial \mathbf{H}(\mathbf{x})}{\partial \mathbf{x}}\right)\right|$$

Find with $h(\mathbf{x})$ adaptive MC techniques: VEGAS [Lepage'78], Parni [Hameren'14],
ML techniques: Normalising Flows Iflow [Bothmann'20] Madnis [Heimel'22], ...

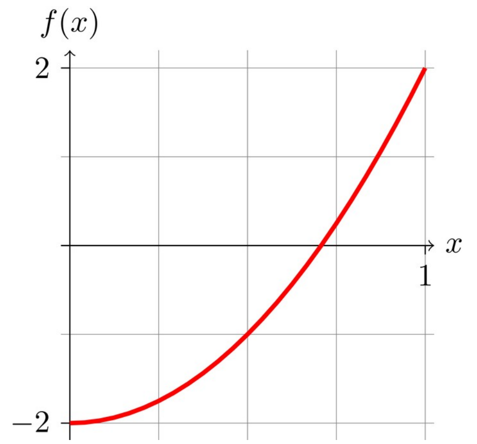
Non-positive definite integrands

- Non-definite integrands introduce computational challenges

  → cancellation between +/- parts increase the variance

- Consider extreme case: $|f(x)|/h(x) = w = \text{const.}$

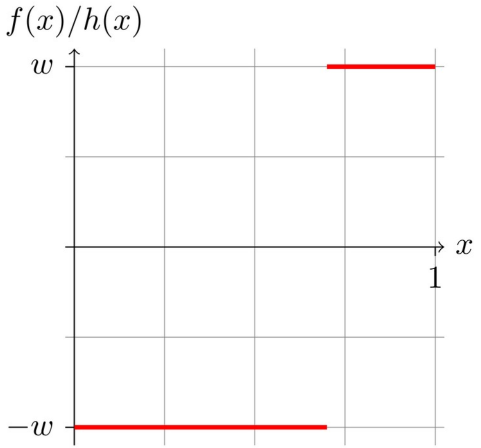
  MC estimate: $\hat{I} = w\frac{N_+ - N_-}{N} \equiv w(2\alpha - 1) \qquad \alpha = N_+/N$



- Lower bound on variance:

$$\mathrm{Var}(\hat{I}) = w^2 - w^2(2\alpha - 1)^2 = w^2(4\alpha(1-\alpha))$$

→ relative uncertainty: $\frac{\delta\hat{I}}{\hat{I}} = \frac{1}{\sqrt{N-1}}\frac{\sqrt{\alpha(1-\alpha)}}{\alpha - \frac{1}{2}}$

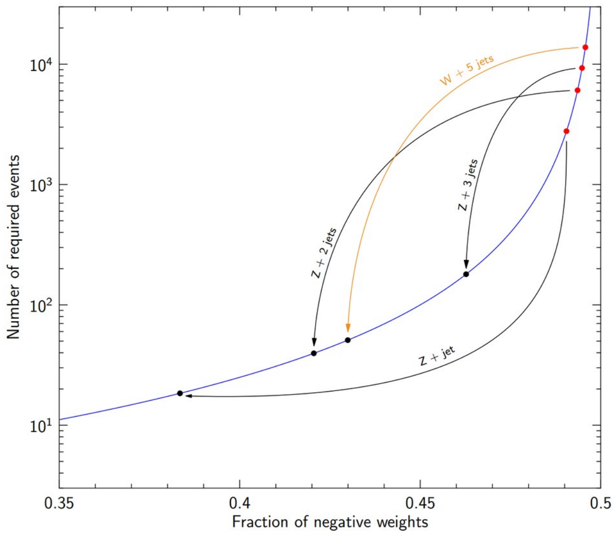


Rephrased: at some point it doesn't matter any more how good your adaptive MC is...

Negative Weights

How to improve convergence
of non-positive definite MC integrals?
→ phase space splitting
[Janssen, Schumann, Poncelet'25]

[Andersen, Maier, Maître, 2023]



How to avoid negative weighted events?
→ Design a positive matching
for example ESME, KrKNLO, …
[van Beekveld, Ravasio, Helliwell, Karlberg, Salam, Scyboz, Soto-Ontoso, Soyez, Zanoli'25]
[Whitehead, Sarmah, Siódmok'24]

I have negative weights
→ How to get rid of them?
Cell-resampling [Anderson, Maier'21]

Current issues

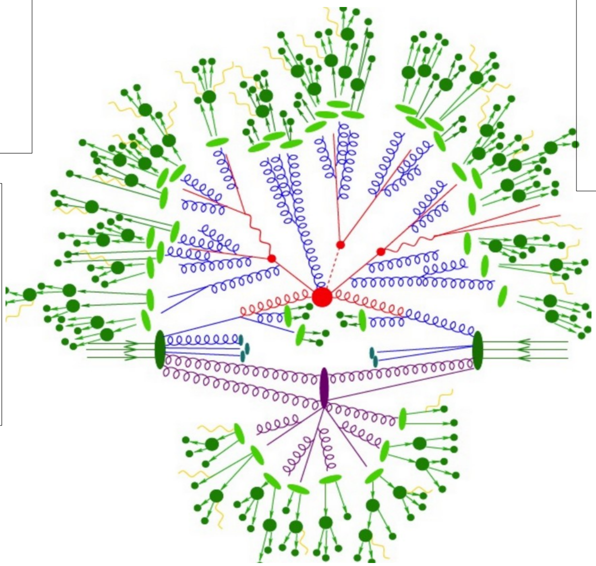
NNLO + PS
→ generality
→ accuracy

Theory uncertainties
→ fixed-order
→ resummation
→ PDFs (aN3LO/flavour schemes)

Mixed EW x QCD corrections
→ amplitudes
→ subtraction

Flavoured jets
→ flavoured algorithms
→ experimental implementation

FO subtraction schemes at NNLO
→ generality & efficiency
→ numerical integration


[Credit: SHERPA]

Toponium/top-pair threshold
→ bound state
→ resummation

Multi-loop amplitudes
→ Methods
→ Automation

...

Summary

Looking forward to a productive week with lots of interesting discussions!