An overview of new(ish) tools for the calculation of scattering amplitudes

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CERN & The University of Edinburgh

Loop-the-Loop, 2024

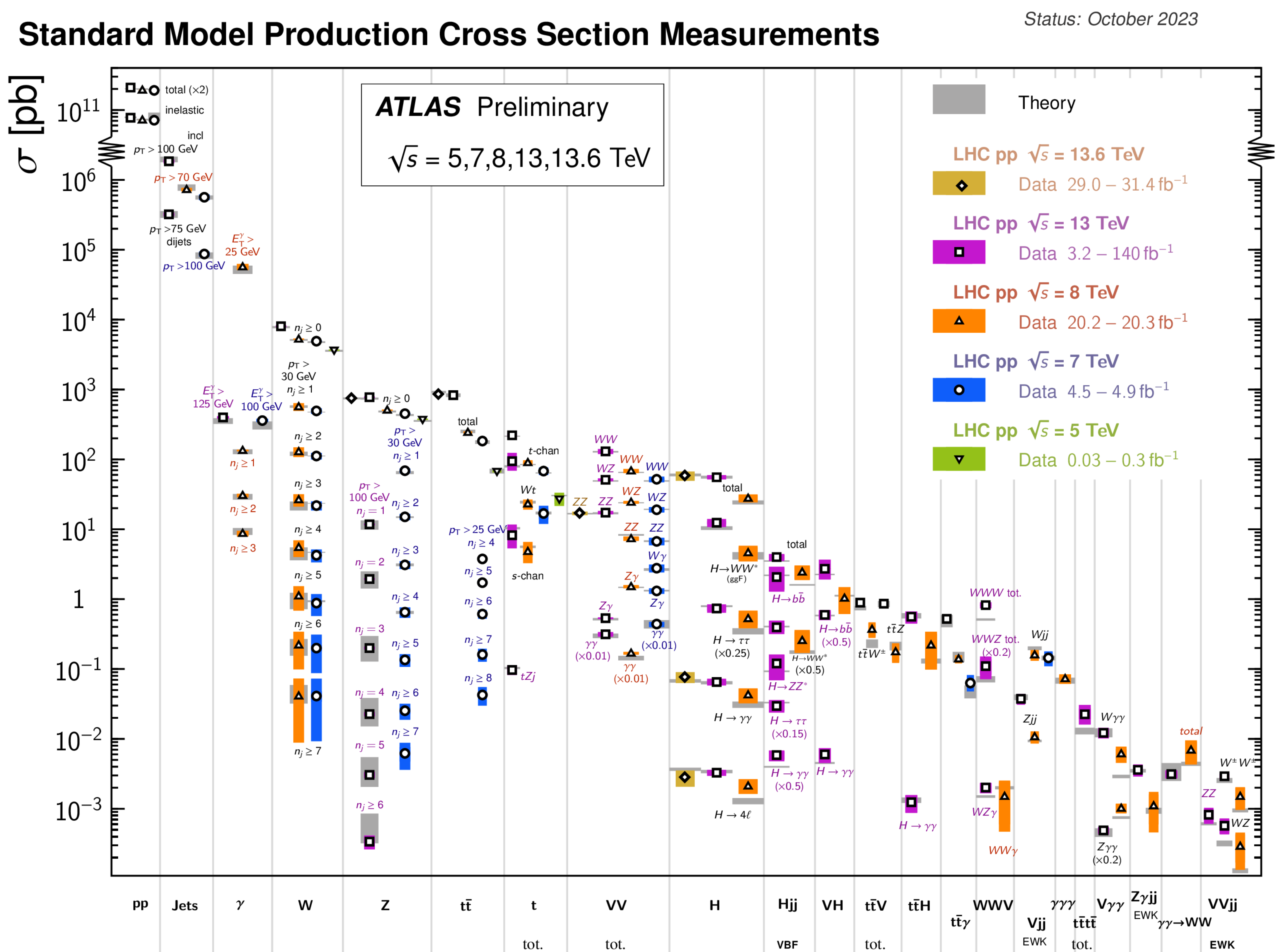
Outline

- Brief overview of theory predictions for collider phenomenology
  - What are the various ingredients that enter these calculations?
- Scattering amplitudes: setup of calculation
- Master integrals
- Master coefficients
- Summary and Outlook

THEORY PREDICTIONS FOR COLLIDER PHENOMENOLOGY

A VERY BRIEF OVERVIEW

Very impressive results in collider physics

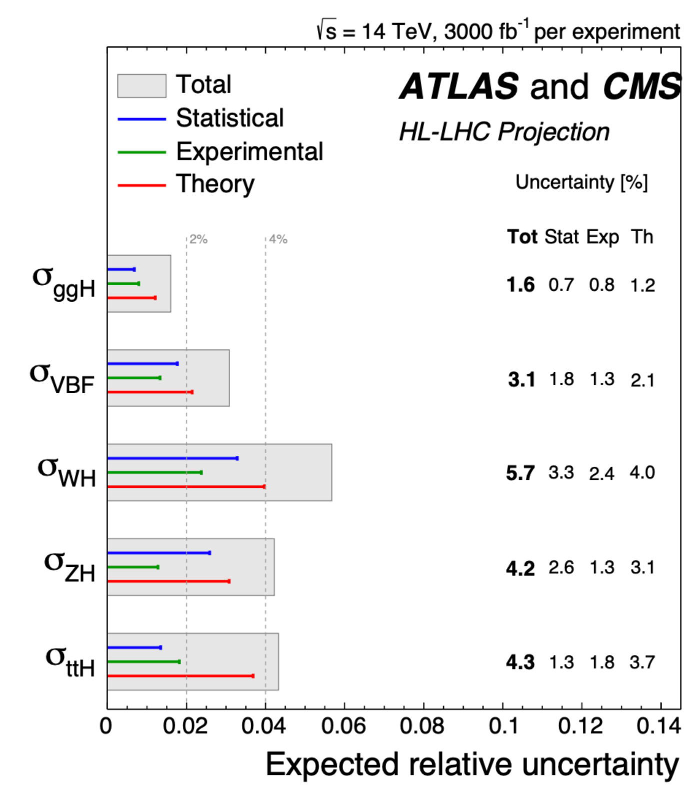


https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PUBNOTES/ATL-PHYS-PUB-2023-039/

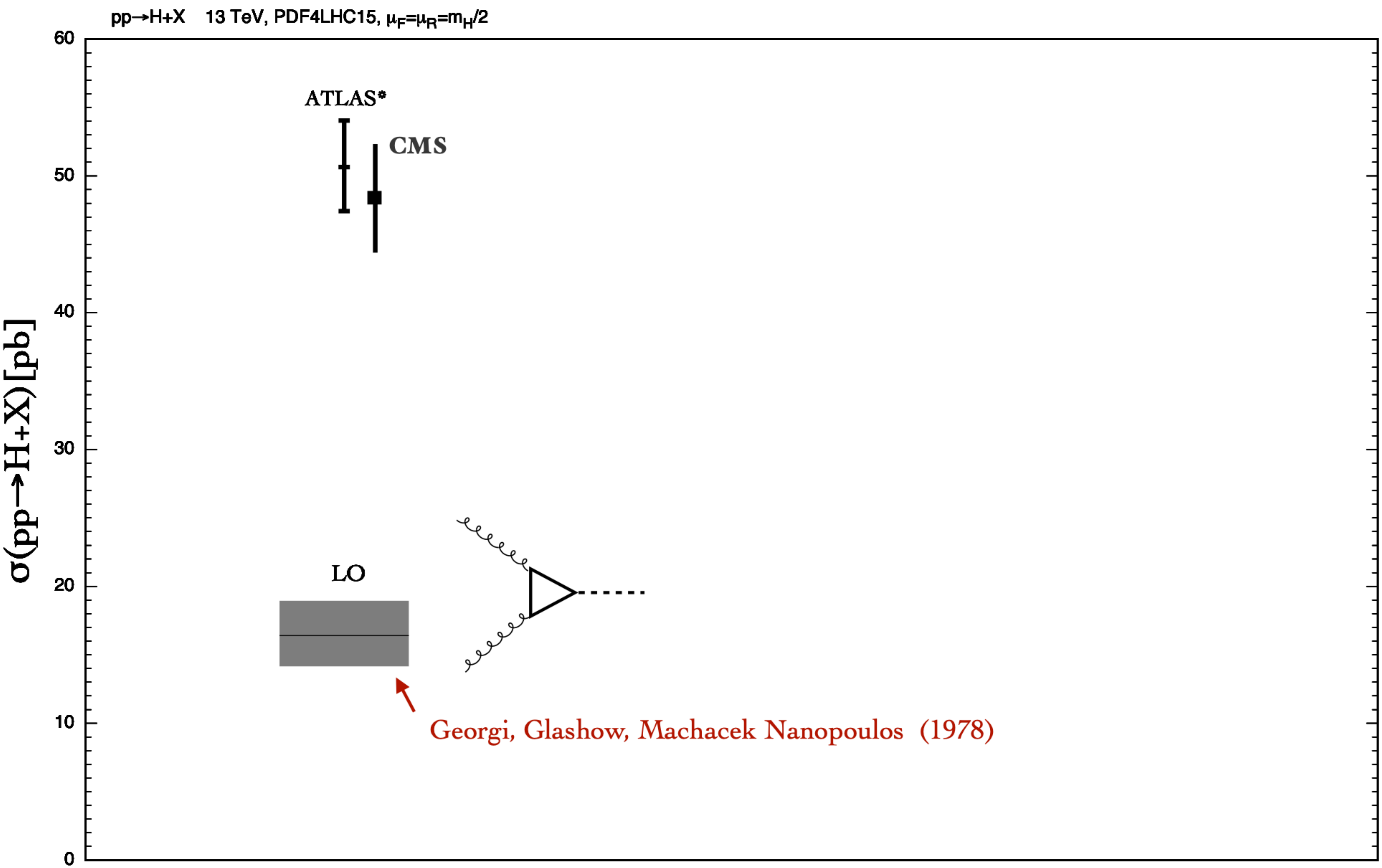
The future —— High-Luminosity LHC

https://hilumilhc.web.cern.ch/content/hl-lhc-project

- ✓ 20 times more data
- ✓ Very high-precision measurements
- ✓ Access to new rare processes
- ✓ Bottleneck in theory predictions…

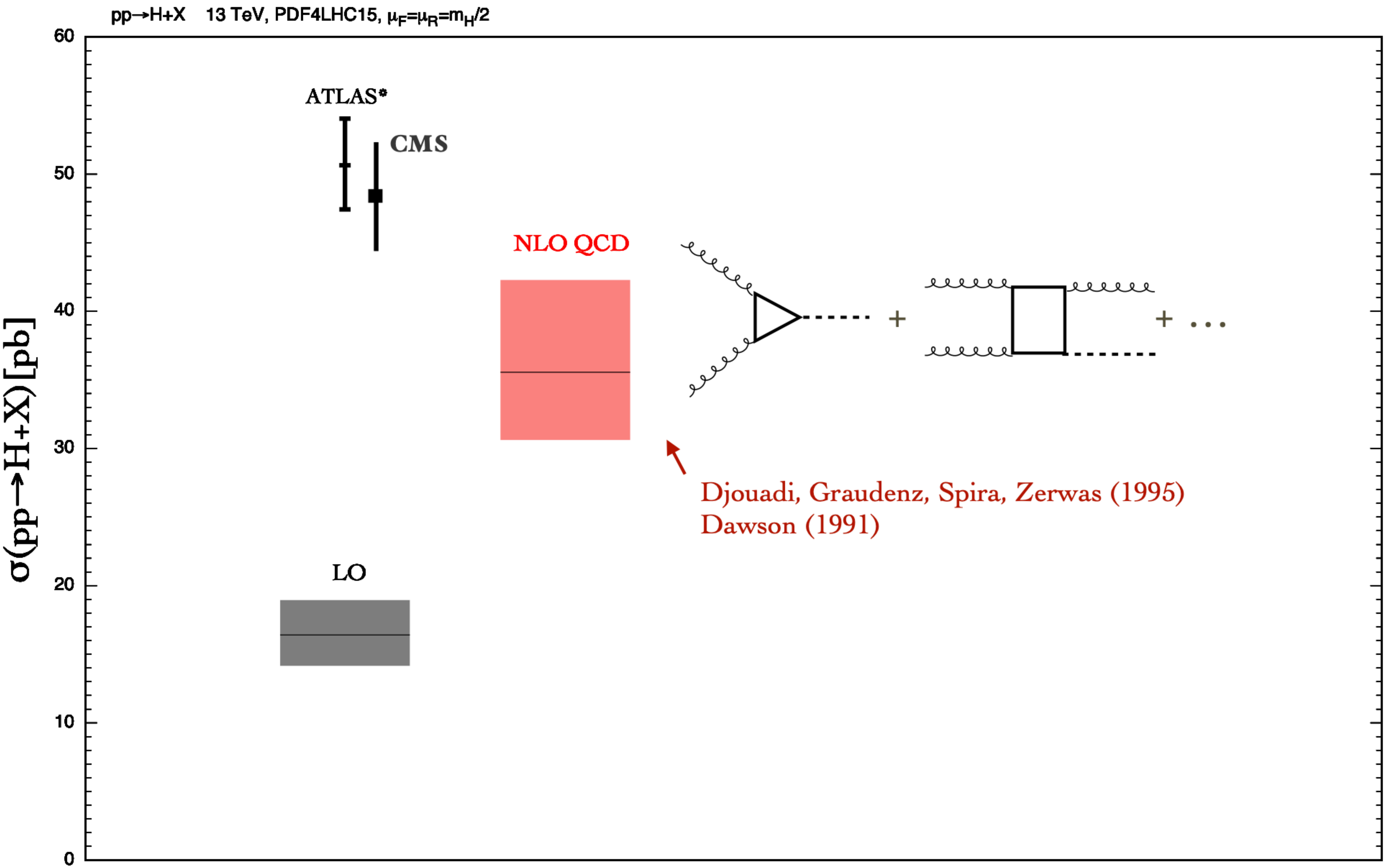


Why do we need precise theory predictions?



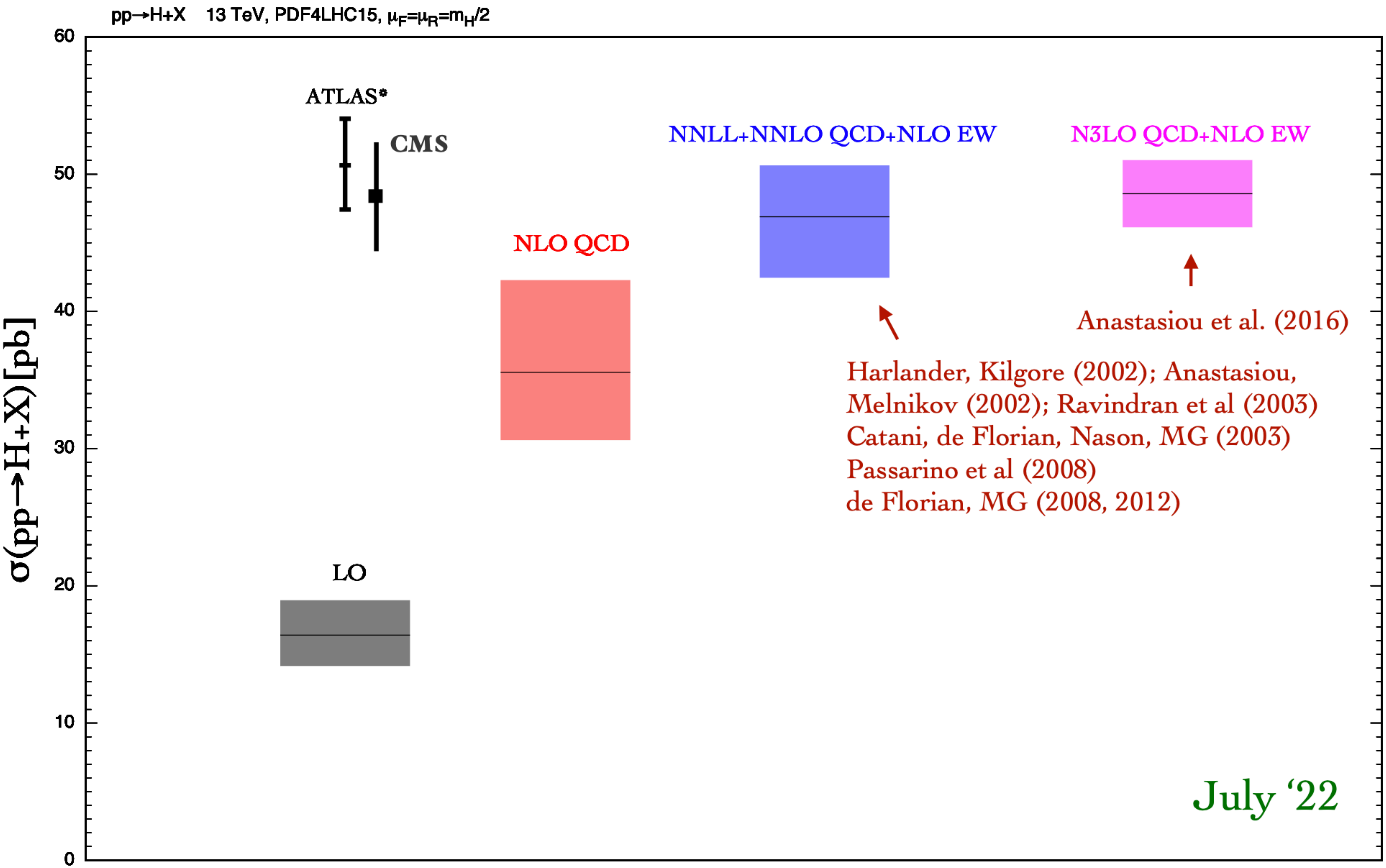
Slide by M.Grazzini

Why do we need precise theory predictions?



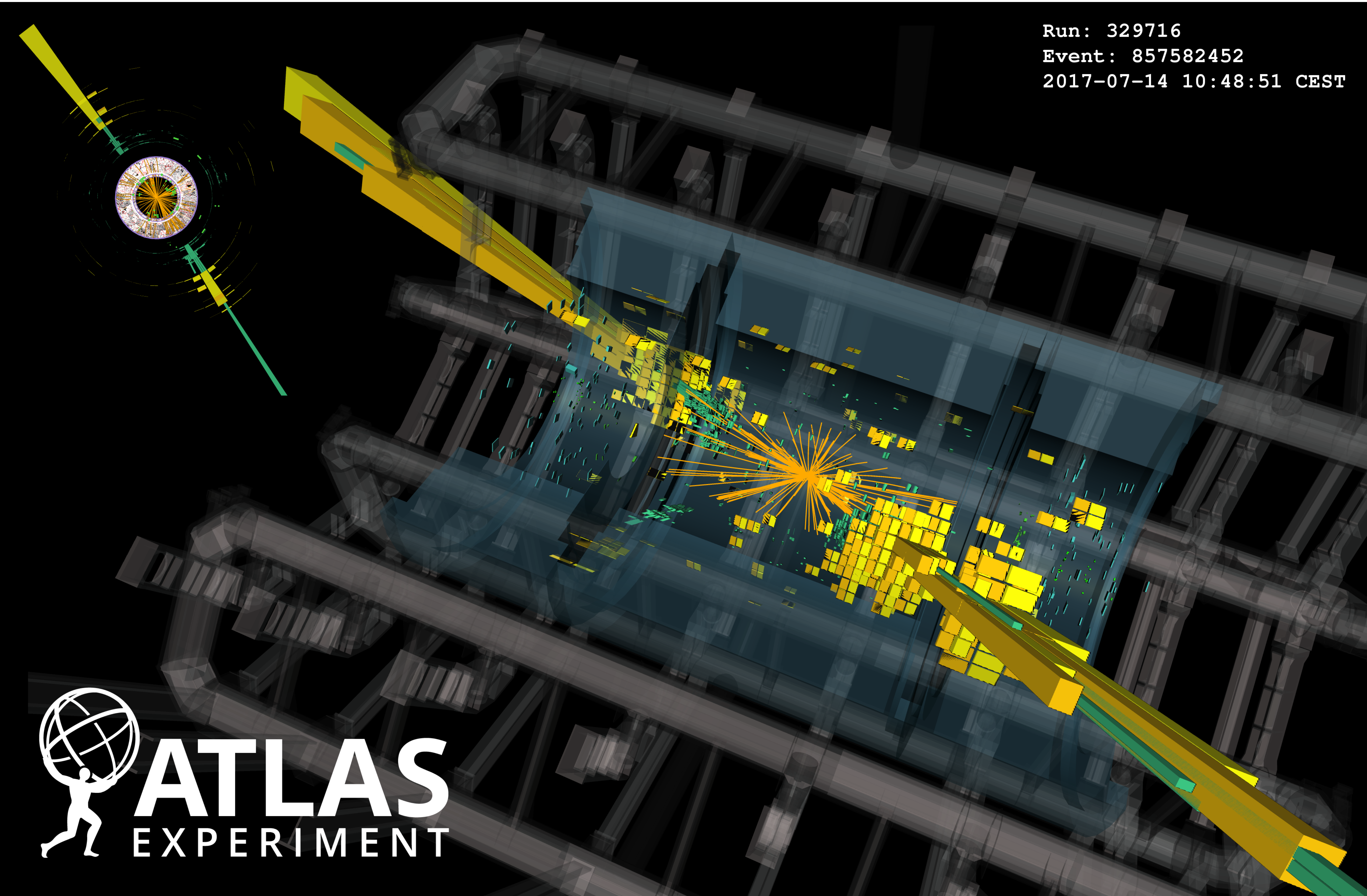
Slide by M.Grazzini

Why do we need precise theory predictions?



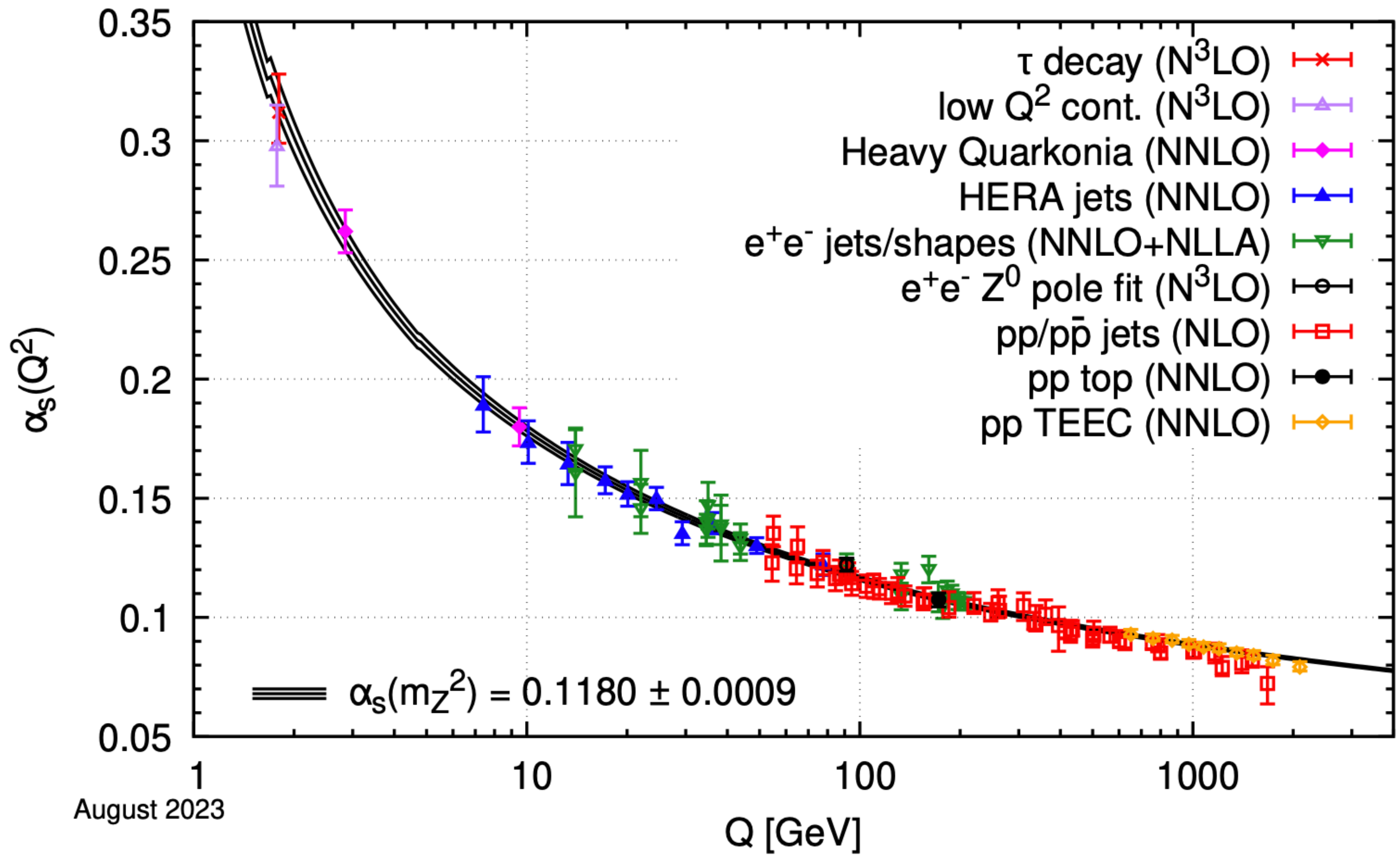
Slide by M.Grazzini

Anatomy of pQCD calculation —— Real Life



Anatomy of pQCD calculation — Scale Dependence

https://pdg.lbl.gov/2023/



- ✓ QCD looks very different at different energies
- ✓ Particles participating in high-energy interactions are not what detectors measure
  - How do we relate the two perspectives?

Anatomy of pQCD calculation — Factorisation

- If sufficiently inclusive over final state (i.e., don't ask too many questions about it)

$$\sigma_{AB\to X} = \sum_{a,b} \int_0^1 dx_a \int_0^1 dx_b \, f_{a|A}(x_a) f_{b|B}(x_b) \, \sigma_{ab\to X}(x_a, x_b) \left(1 + \mathcal{O}(\Lambda_{QCD}/Q)\right)$$

Parton Distribution Functions (PDFs): non perturbative, but universal

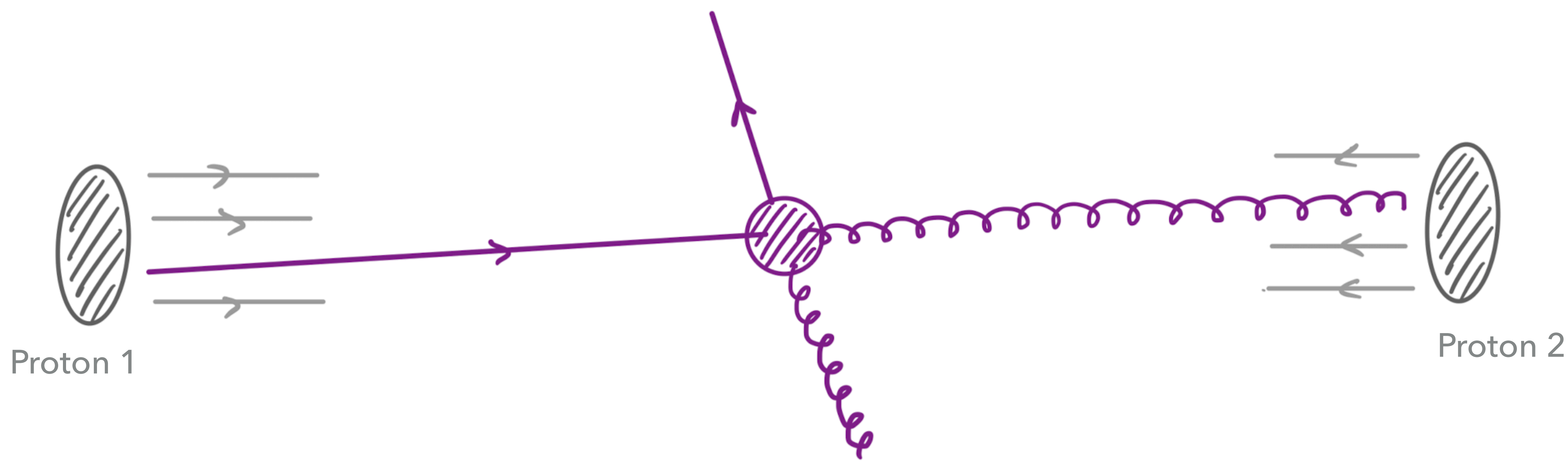
Hard scattering: perturbation theory

Non-perturbative effects: power suppressed

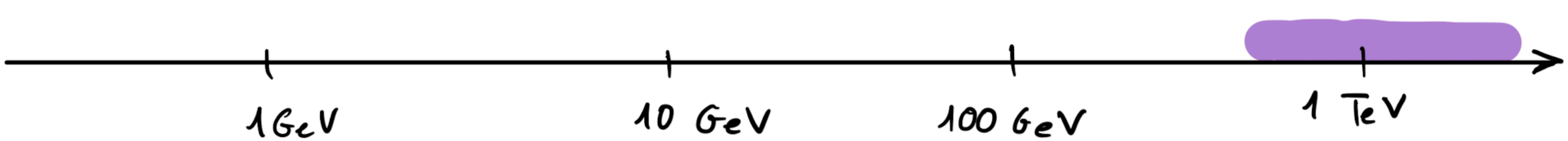
- Collinear factorisation
  - Can define a universal object (the proton) and measure its distribution of quarks and gluons
- Asymptotic freedom: at high-energies, the theory is perturbative
  - Can compute the hard scattering in perturbation theory
- Non-perturbative corrections to factorisation formula: largely unstudied…
  - Start to become an obstruction to increase of theory precision

Anatomy of pQCD calculation — Hard Interaction

- ✓ A high-energy parton is extracted from each proton
  - Rely on non-perturbative PDFs to describe the proton

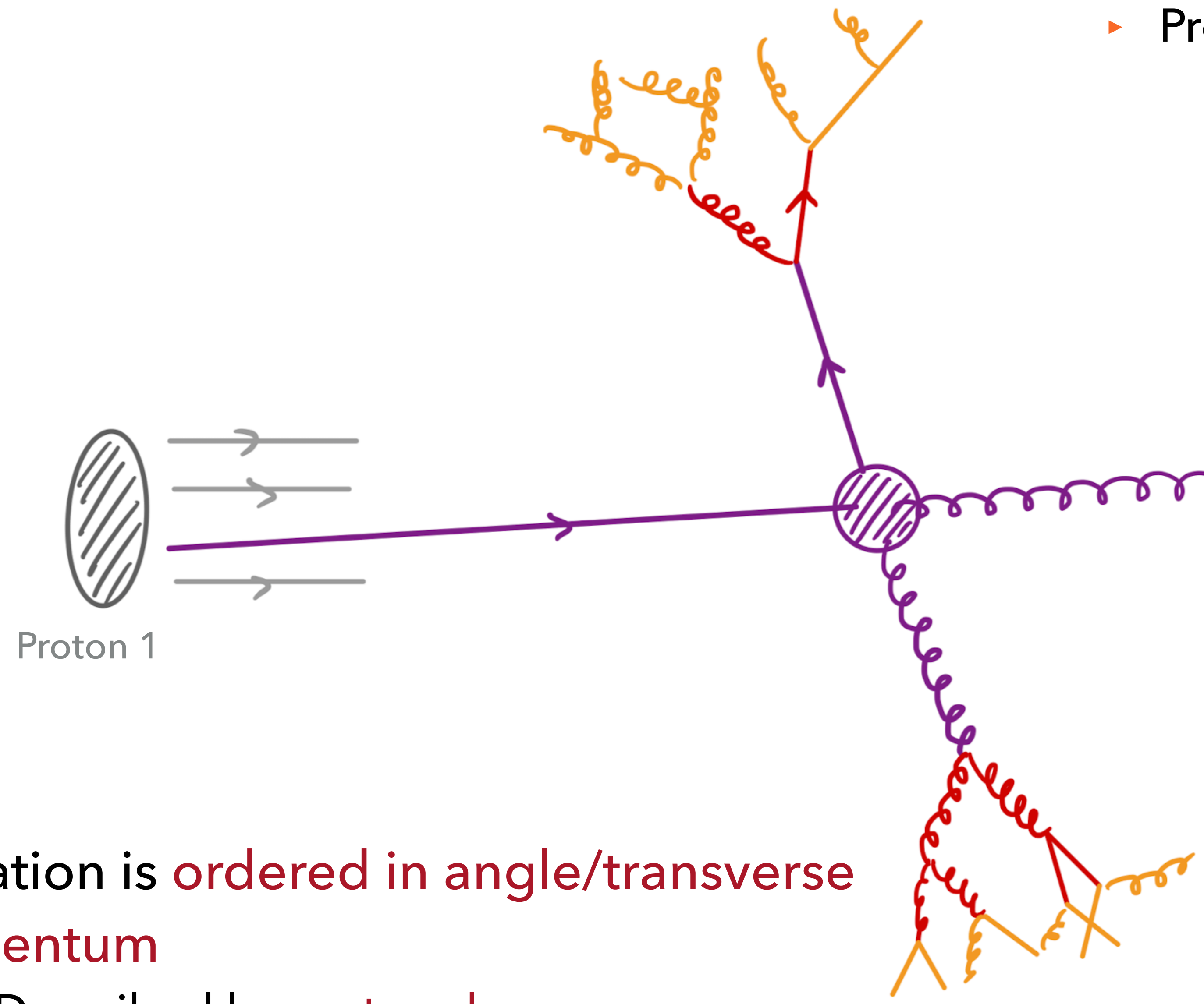


- ✓ High-energy interaction:
  - Computable in perturbative QCD ⇒ Amplitudes!
  - Produce high-energy particles

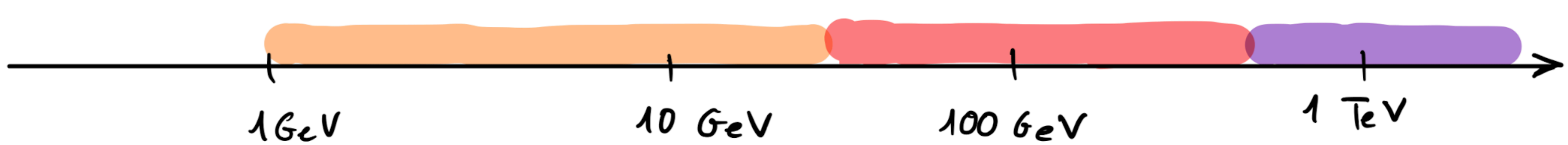


Anatomy of pQCD calculation — Parton Showers

- ✓ Particles produced in the final state radiate
  - Proliferation of particles fill phase-space

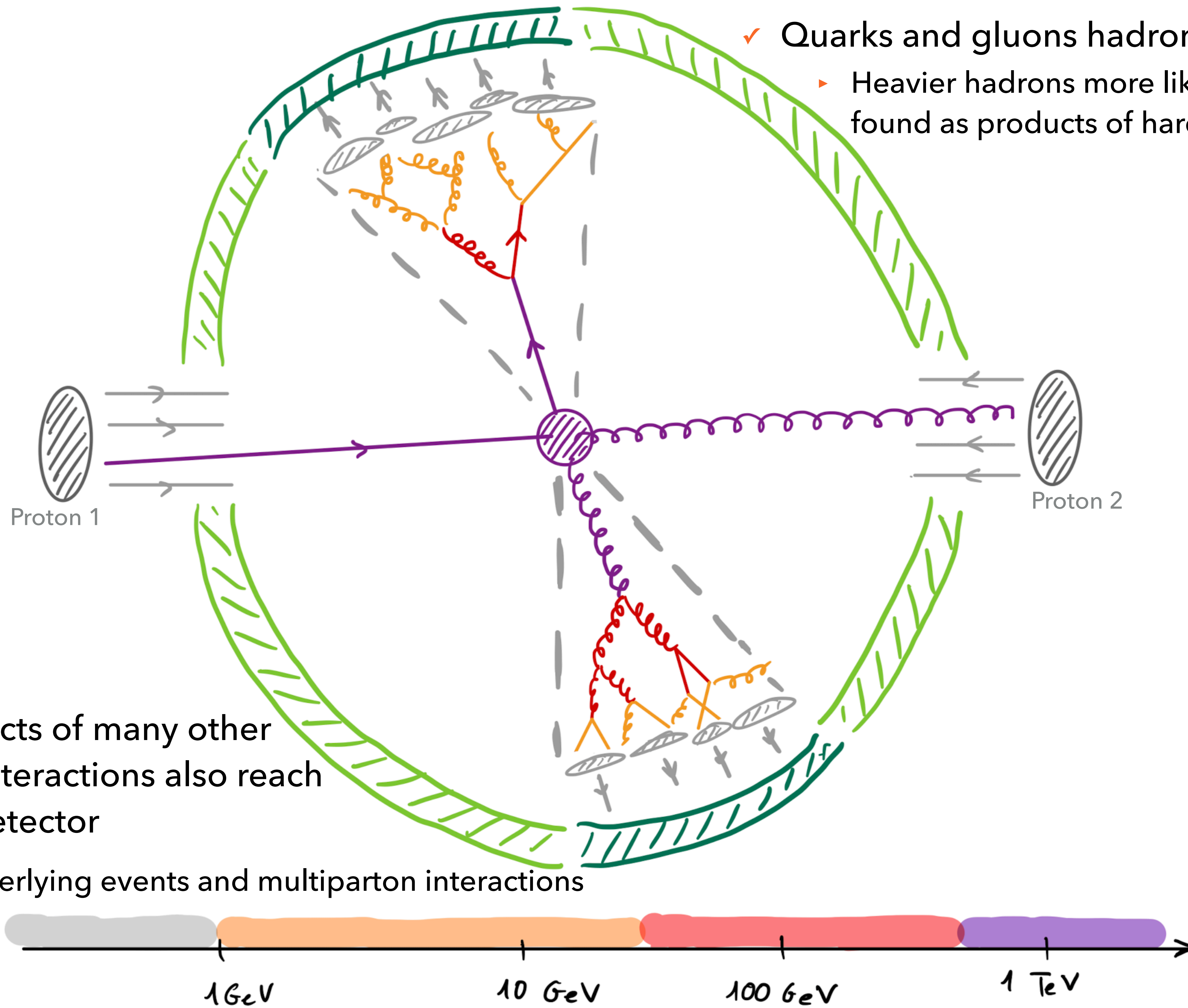


- ✓ Radiation is ordered in angle/transverse momentum
  - Described by parton showers
  - Form collimated jets of particles



Anatomy of pQCD calculation — Hadronisation and UE&MPIs

- ✓ Quarks and gluons hadronise
  - Heavier hadrons more likely to be found as products of hard interaction



- ✓ Products of many other soft interactions also reach the detector
  - Underlying events and multiparton interactions

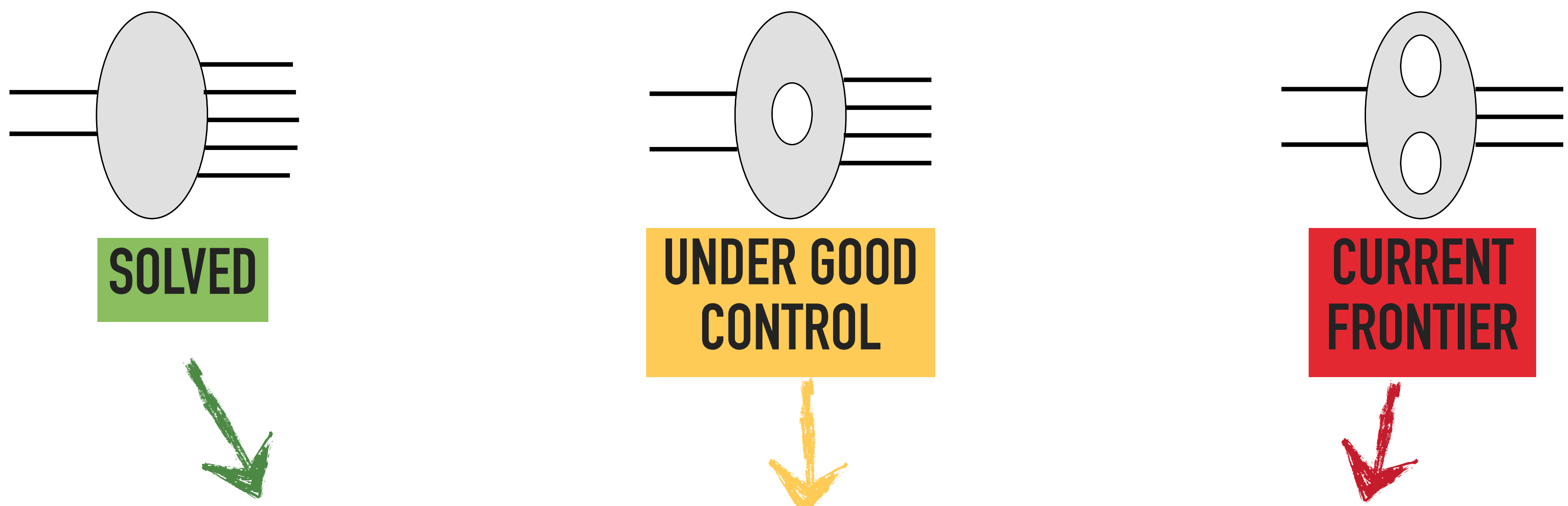
Hard Interactions

- Percent-level precision for several observables

$$\sigma = \sigma_{LO}\left(1 + \alpha_s \sigma_{NLO} + \alpha_s^2 \sigma_{NNLO}\right) + \mathcal{O}(\alpha_s^3)$$

$\sim \mathcal{O}(10\%)$ $\qquad \sim \mathcal{O}(1\%)$

- Amplitudes for NNLO corrections (five-point processes)



$$\sigma_{NNLO} = \sigma_{RR} + \sigma_{RV} + \sigma_{VV}$$

- Factorisation of work: amplitudes and phase-space integration

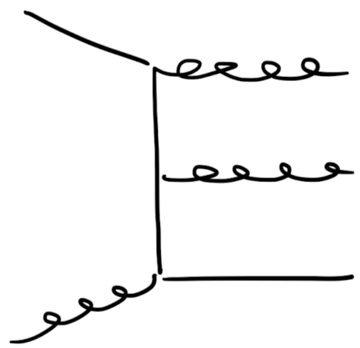
$$\sigma \sim \int d\Phi \, |\mathcal{A}|^2$$

NB: Divergences appear, work in Dimensional Regularisation, $4 \to D = 4 - 2\epsilon$

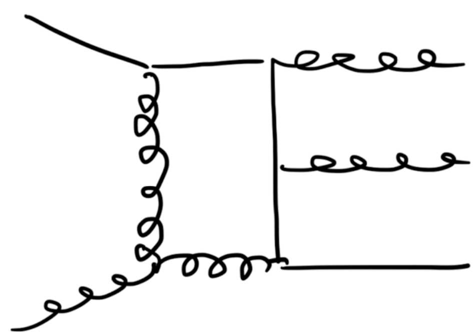
Loops and Legs

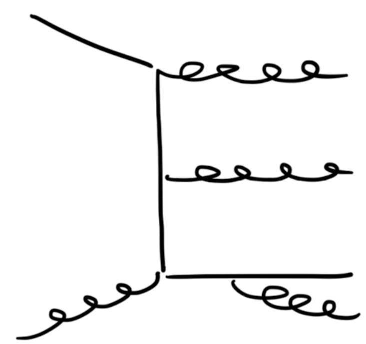
$$\sigma \sim \int \mathrm{d}\Phi \, \left|\mathscr{A}\right|^2$$

Leading Order

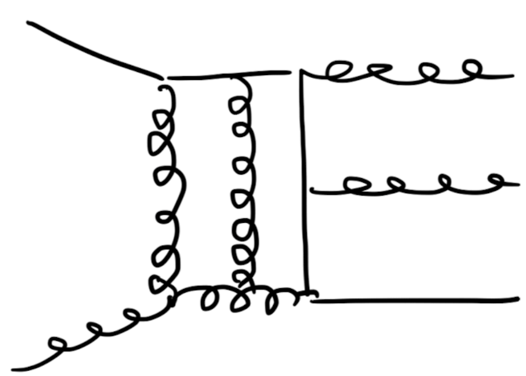


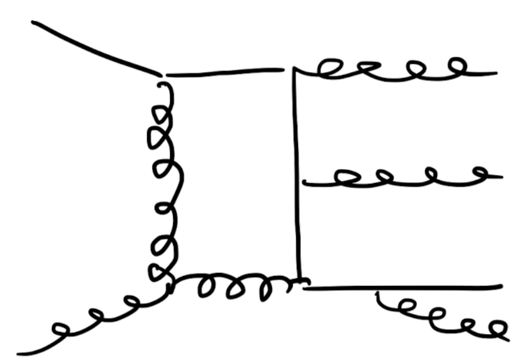
NLO

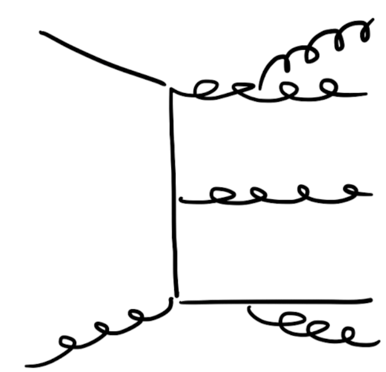




NNLO





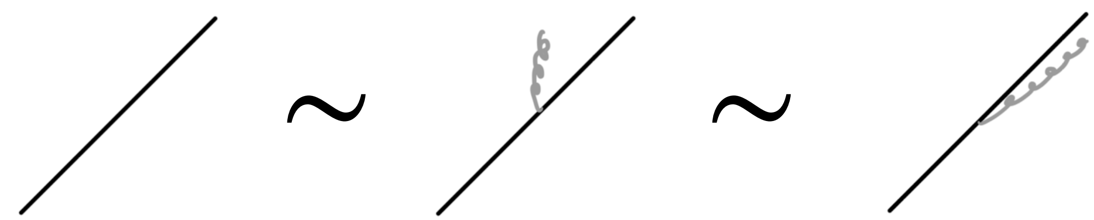


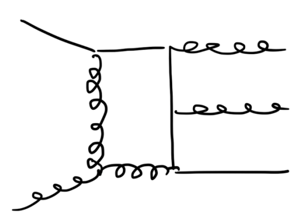
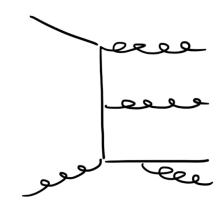
- ✓ The higher the order, the more loops and external legs we have

Phase-space integration and singularities

$$\sigma \sim \int d\Phi \, \left|\mathscr{A}\right|^2$$

- ✓ Loop amplitudes have IR singularities (after UV renormalisation)
- ✓ Phase-space integration has IR singularities



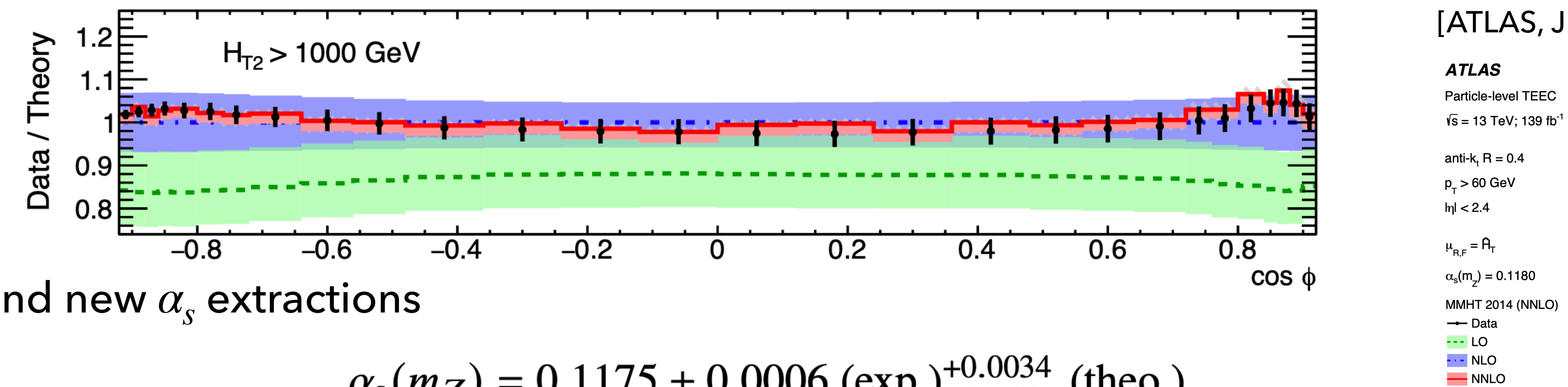
- ✓ Sum is finite: $\int d\Phi_3$  $+ \int d\Phi_4$ 
- ✓ Two approaches in phase-space integration:
  - Subtraction: build counter terms ⇒ process specific, very efficient
  - Slicing: introduce cut-off in integration ⇒ process independent, less efficient
- ✓ See subtraction talks this afternoon [talks by Gloria, Federica]
- ✓ And a different way to combine things to avoid it [talk by Matilde]

Anatomy of pQCD calculation — Summary

- Need ever more precise theoretical predictions to make the most out of experimental data
- Theoretical predictions for collider processes involve many components
  - ✓ Need efficient and precise codes for each of these components
- Example: NNLO corrections to 3-jet production at the LHC
  - Energy-energy correlators…

[Czakon, Mitov, Poncelet '21]

[ATLAS, JHEP 07 (2023) 85]



  - … and new α_s extractions

$$\alpha_s(m_Z) = 0.1175 \pm 0.0006\ (\text{exp.})^{+0.0034}_{-0.0017}\ (\text{theo.})$$

  - Among most complex NNLO calculations: 100M CPU hours (~700 tons of CO2!) ⇒ big problem we need to address for the future!
- Keep these challenges in mind when declaring an amplitude solved

SCATTERING AMPLITUDES

SETUP OF CALCULATION (FOCUS ON MULTILEG PROCESSES)

Master integral decomposition

$$\mathscr{A} = \sum c_i(\vec{p};\epsilon)\; m_i(\vec{p};\epsilon)$$

Master coefficients
- process specific
- rational/algebraic functions

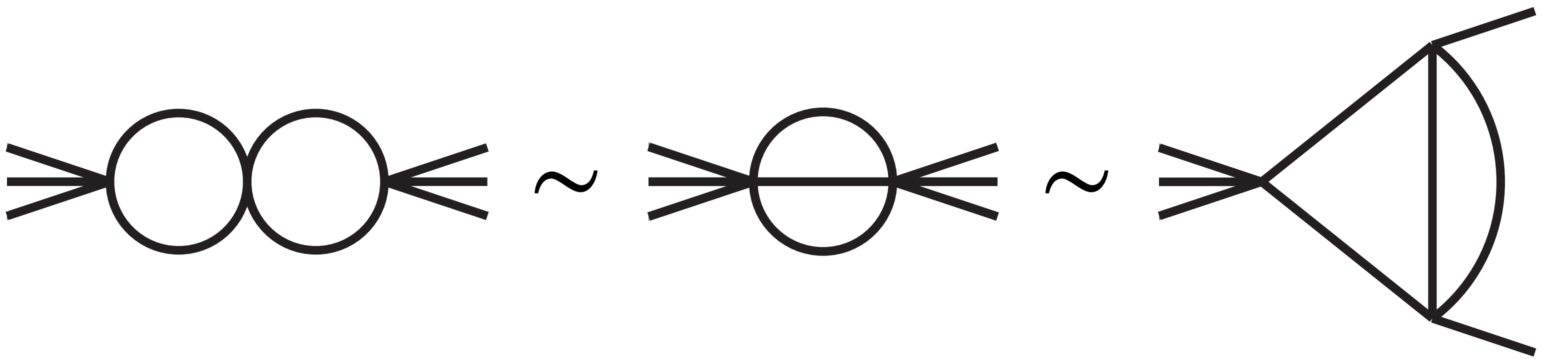
Master integrals
- kinematic dependent
- special functions (polylogs, elliptics, …)

- How?
  - ✓ construct amplitude integrand (QGRAF+projectors, Generalised Unitarity, …)
  - ✓ IBP reduce (Blade, FiniteFlow, Fire, Kira, LiteRed, NeatIBP, Reduze, …)
- Extremely complicated coefficients, even with “good basis”
- Decomposition valid to all orders in ϵ …
- … but we only care about the first orders

} Can we use this to simplify our life?

Bases of Special Functions

- Relations after expansion in ϵ:



$$\sim r_0 + r_1\,\epsilon\,\ln(s) + r_2\,\epsilon^2\,\ln^2(s) + \ldots$$

- Make relations explicit: basis of transcendental functions at each order

$$\mathscr{A} = \sum c_i(\vec{p};\epsilon)\; m_i(\vec{p};\epsilon)$$

$$m(\vec{p}) = \sum \epsilon^j\, h_j(\vec{p})$$

$$\Downarrow$$

$$\mathscr{A} = \sum \epsilon^j \sum d_{j,k}(\vec{p})\; h_k(\vec{p})$$

[Gehrmann, Henn, Lo Presti, 18]
[Chicherin, Sotnikov, 20]
[Chicherin, Sotnikov, Zoia, 21]
[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, Zoia, 23]
[Gehrmann et al 24]

Setup of Calculation

$$\mathscr{A} = \sum \epsilon^j \sum d_{j,k}(\vec{p})\ h_k(\vec{p})$$

1. Master integrals:
   - ✓ Decompose in terms of special functions
   - ✓ Efficient and stable numerical evaluation to required order in ϵ
   - ✓ Pick basis that manifest analytic properties of amplitudes

2. Coefficients
   - ✓ Directly compute coefficients in ϵ expansion
   - ✓ Simplify for efficient and stable numerical evaluation

MASTER INTEGRALS

SPECIAL FUNCTIONS AND NUMERICAL EVALUATION

Master Integrals I

- How to compute them? Many ways…
  - ✓ Identify independent transcendental components
  - ✓ Convenient representation for fast/stable numerical evaluation

- Differential equations in canonical form

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

$$d\vec{M} = \epsilon \, A \, \vec{M} \qquad\qquad A(\vec{p}) = \sum A_i \;\, d \ln W_i(\vec{p})$$

  - ✓ Find special (pure) basis
  - ✓ W_i $\Rightarrow$ "symbol alphabet": analytic information, in usable form

Master Integrals II

$$d\vec{M} = \epsilon\, A\, \vec{M} \qquad\qquad A(\vec{p}) = \sum A_i \;\, d\ln W_i(\vec{p})$$

- Finding pure basis
  - ✓ Several semi-automated methods, but not yet systematic
- Finding the symbol alphabet
  - ✓ Special points in phase space: Landau analysis

[talks by Maria, Mathieu, …]

All investigations done with finite field numerical evaluations

[FiniteFlow, Fire, Kira, …]

[Schabinger, von Manteuffel, 14]
[Peraro, 16]

- Finding the constant matrices A_i
  - ✓ Rational numbers: use numerical evaluations
  - ✓ Trivial once pure basis and alphabet known

Master Integrals III — (Analytic) Solution

$$d\vec{M} = \epsilon\, A\, \vec{M} \qquad\qquad A(\vec{p}) = \sum A_i \; d\ln W_i(\vec{p})$$

- Solve order by order $\quad m(\vec{p}) = \sum \epsilon^j\, h_j(\vec{p})$

- Multiple Polylogarithms
  - ✓ Cumbersome representation, region specific
  - ✓ Relations not explicit
  - ✓ Use Ginac for evaluation, but slow…

- Chen iterated integrals
  - ✓ Relations are explicit
  - ✓ Write dedicated code for evaluation

[Chicherin, Sotnikov, 20]
[Chicherin, Sotnikov, Zoia, 21]
[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, Zoia, 23]

- Numeric alternatives: currently too slow, but potential for interpolation
  - ✓ pySecDec [Heinrich et al 15, 17, 18, 21,23, 24…]
  - ✓ Series Expansion [Moriello 19] [Hidding 20] [Armadillo et al 22]
  - ✓ AMFlow [Liu, Ma, (Wang), (17), 21, 22]

COEFFICIENTS

COMPUTATION AND SIMPLIFICATION

Coefficients I

$$\mathscr{A} = \sum \epsilon^j \sum d_{j,k}(\vec{p})\ h_k(\vec{p})$$

- Now that the h_k are known, determine $d_{j,k}$

- Strategy: Ansatz constrained by (finite field) numerical evaluations

$$d(\vec{p}) = \frac{\mathscr{N}(\vec{p})}{\mathscr{D}(\vec{p})}$$

[Schabinger, von Manteuffel, 14]
[Peraro, 16]

  - ✓ Numerator/Denominator are polynomials of high degree
  - ✓ Generate the "numerical data"

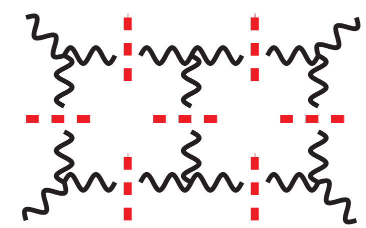
Coefficients II — "Numerical data"

"Feynman diagrammatic"

- ✓ Generate integrand: QGRAF, …
- ✓ Project on form factors
- ✓ IBP reduce (with syzygy, block triangular, …)

"Two-loop generalised unitarity"

- ✓ Parametrise generic integrand as surface terms/master integrands
- ✓ Generate integrand: product of trees



Caravel

$$\mathscr{A}(p_0) = \sum c_i(\vec{p}_0; \epsilon)\ m_i(\vec{p}; \epsilon)$$

- ✦ Almost done:

$$\mathscr{A}_0 = \mathscr{A}(p_0)\ /.\ \left\{ m_i(\vec{p}) \to \sum \epsilon^j\, h_j(\vec{p}) \right\} \Longrightarrow \boxed{\mathscr{A}_0 = \sum \epsilon^j \sum d_{j,k}(\vec{p}_0)\, h_k(\vec{p})}$$

Coefficients III — Fitting coefficients

$$d(\vec{p}) = \frac{\mathcal{N}(\vec{p})}{\mathcal{D}(\vec{p})}$$

[Badger et al]

[von Manteuffel et al]

[Ita et al]

- Denominator: essentially nothing to do if you have the integrals!

$$\mathcal{D}(\vec{p}) = \prod W_i^k$$

- Much simpler problem (but still hard): only need $\mathcal{N}(\vec{p})$!
  - Morally easy: determine a polynomial from exact numerical data
  - Algorithms scale very badly with degree/number of variables
  - Many ways to improve performance, very important in practice:
    - Univariate slices
    - Univariate/multivariate partial fractions
    - Choice of variables
    - p-adic numbers

Coefficients IV — Clean up and Assembly

$$\mathscr{A} = \sum \epsilon^j \sum d_{j,k}(\vec{p})\ h_k(\vec{p})$$

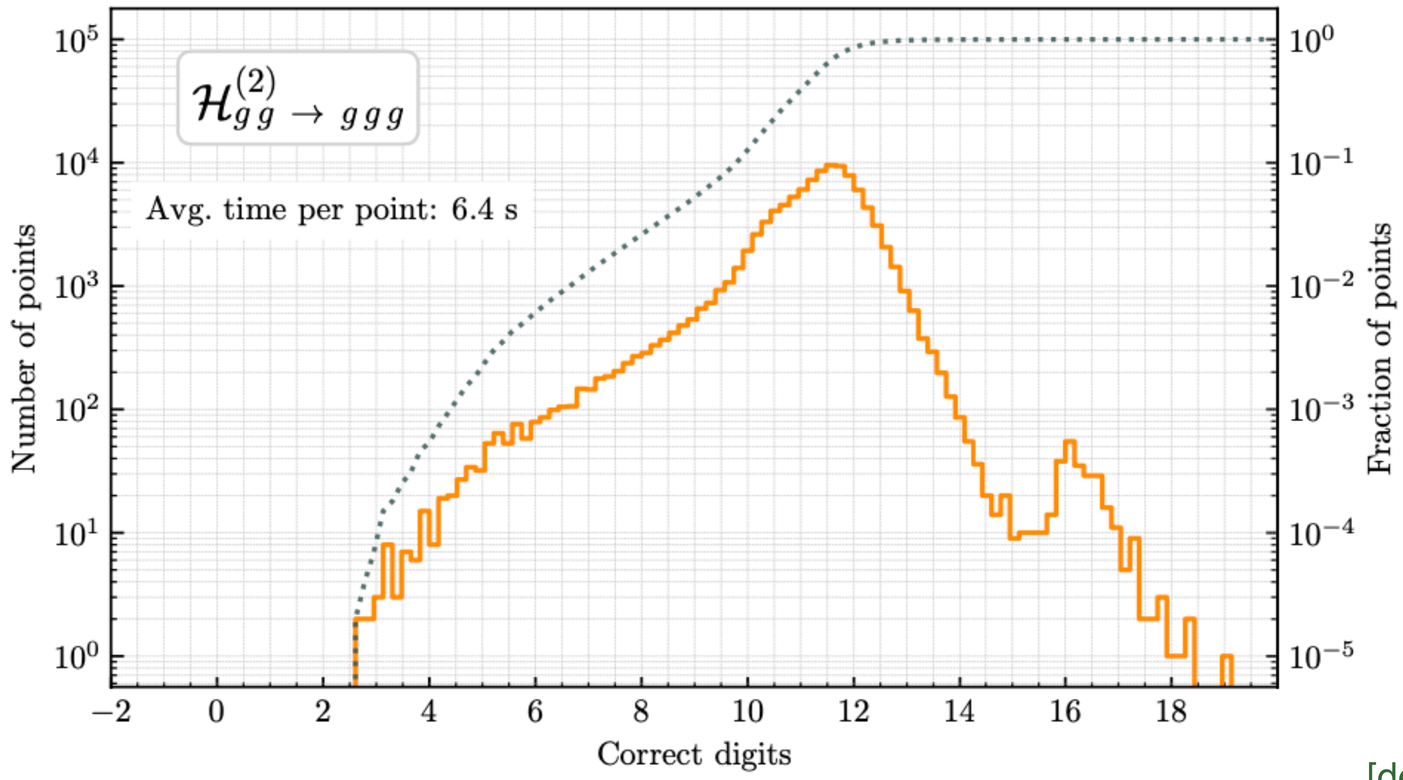
- Important for pheno-ready results
- Assemble full amplitude: all colour structures/permutations/channels
  - ✓ Large combinatorial factors…
- Most $d_{j,k}$ are related ⇒ write in basis of rational functions
- Clean-up basis for fast evaluation
  - ✓ Multivariate partial fractions
  - ✓ Pick the right variables!
- Implement everything in C++ code
  - ✓ Precision rescue system: hiding in the symbol alphabet (cheap!)

[e.g., Abreu, Page, Pascual, Sotnikov, 20]

SUMMARY AND OUTLOOK

Summary and Outlook

- Amplitudes for two-loop five-point massless processes
  - 2013: first numerical results, all-plus gluon, 4/5 digits
  - 2017: compute them at a single (unphysical) phase-space point in $\mathcal{O}$(10mins)
  - 2018/2019: first analytic results for planar corrections, $\mathcal{O}$(50MB) text files for c_i
  - 2022/2023: completed all two-loop five-point massless processes for the LHC
  - Compact and efficient expressions: $\mathcal{O}$(1s)/point, expressions printed in papers



[de Laurentis et al, 23]

Summary and Outlook

- A lot of progress in techniques for computing amplitudes
  - ✓ Tied to progress on calculation of Feynman integrals [all talks on Monday, **Sara** and **Sebastian's** talks today]
- Important applications for particle pheno, gravity, formal studies
- Many things I did not discuss
  - ✓ Techniques for amplitudes with fewer legs/internal masses [see e.g. **Tommaso's** talk on Monday, **Federico's** today]
  - ✓ Expansions and approximations
  - ✓ Do we actually need exact higher order amplitudes? Sometimes no… $pp \to Ht\bar{t}, pp \to Wt\bar{t}$ [Catani et al, 22 ; Buonocore et al 23]
- Adding internal masses: top physics, EW corrections, … [see **Colomba's** talk]
- Towards NNNLO $\Rightarrow$ more loops! [see **Dhimiter** and **Junwon's** talks]

THANK YOU!