

Multi-loop calculations and computing for precision physics at the LHC



Robert M. Schabinger
Michigan State University

The Big Picture

Fundamental Large Hadron Collider Processes

- Strong Corrections to Gluon-Fusion Higgs Production

- Strong Corrections to Drell-Yan Lepton Production

Efficient Computer Algebra for Multi-Loop Calculations

- Efficient Integration by Parts Reduction

- Phenomenological Ramifications

Computing, Scientific Software, and Machine Learning

- Computing

- Scientific Software

- Machine Learning

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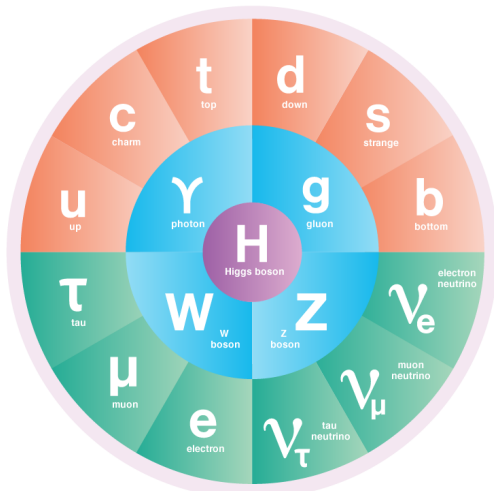
Computing, Scientific Software, and Machine Learning

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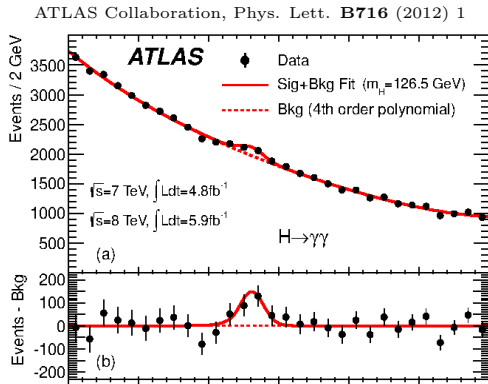
The Standard Model of Particle Physics

Microscopic model, a renormalizable quantum field theory.



Consider the 2012 Higgs Boson Discovery @ LHC

Decades of experimental and theoretical work to produce *e.g.*



On the theory side, predict (as a function of s and M_h):

1. How many Higgs bosons are produced?
2. What are the measurable decay modes of the Higgs?
3. What other interactions mimic these Higgs events?



Cross Sections in the Standard Model

For simplicity, focus on Higgs **production**. How do I estimate the total number of Higgs bosons I expect to produce after running the LHC for a fixed amount of time?

1. Calculate the *cross section*, σ , or the probability that the colliding protons produce a Higgs boson per unit time, divided by the particle flux density of the LHC.
2. The *integrated luminosity*, $\int L dt$, is the particle flux density integrated over the time of data acquisition.
3. The number of events in the sample is then $\sigma \int L dt$.

Cross section calculations in the Standard Model are key!



Technical Complications of Perturbative Calculations

Beyond leading order, severe technical complications for \mathcal{M}

$$\mathcal{M}(q(p_1)\bar{q}(p_2)\rightarrow\mu(p_3)\bar{\mu}(p_4)) = \text{tree} + \text{loop} + \dots$$

- ▶ Feynman diagrams which contain loops lead to ill-defined integrals over the four-momenta of virtual quanta.
- ▶ Only **ultraviolet divergences** coming from large values of the loop momenta are subject to renormalization.
- ▶ For remaining **infrared divergences**, add higher-multiplicity scattering processes at the same relative order in α_s , *e.g.*

$$\mathcal{M}(q(p_1)\bar{q}(p_2)\rightarrow\mu(p_3)\bar{\mu}(p_4)g(k)) = \text{tree} + \text{loop} + \dots$$

Need consistent manipulations of divergent integrals!



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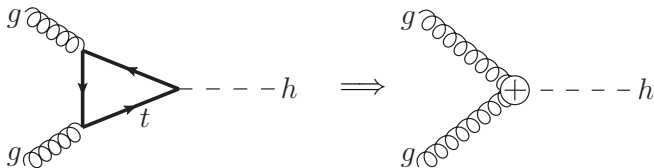
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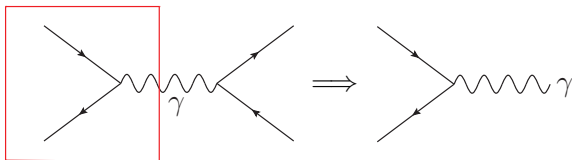


Gluon-Fusion Higgs and Drell-Yan Lepton Production



Surprisingly, the most important source of Higgs bosons @ LHC.

Georgi *et. al.*, Phys. Rev. Lett. **40** (1978) 692



Clean experimentally, very useful to constrain the probability of finding a quark or gluon of a specified energy inside the proton.

Drell and Yan, Phys. Rev. Lett. **25** (1970) 316

First Higgs and Drell-Yan Predictions At $\mathcal{O}(\alpha_s^3)$

C. Anastasiou *et. al.*, Phys. Lett. **B737** (2014) 325;

Y. Li, A. von Manteuffel, **RMS**, and H. X. Zhu, Phys. Rev. **D91** (2015) 036008

$$\lim_{\hat{s} \rightarrow M_i^2} \left\{ \Delta \hat{\sigma}_i^{\text{N}^3\text{LO}} \right\} = H_i S_i, \text{ where } i = h \text{ or } \gamma$$



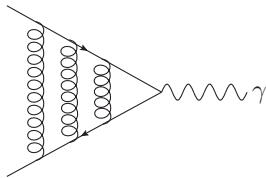
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H_i **hard**, effects due to virtual quanta:



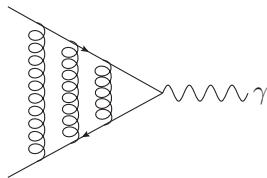
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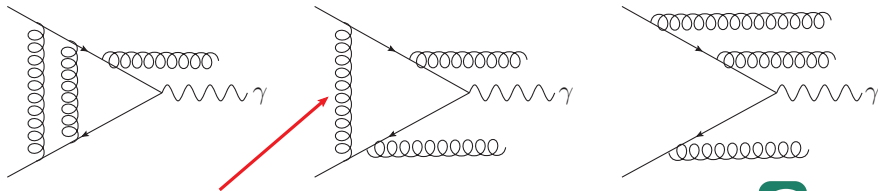
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H_i **hard**, effects due to virtual quanta:



S_i **soft**, effects due to real radiation, soft to first approximation:

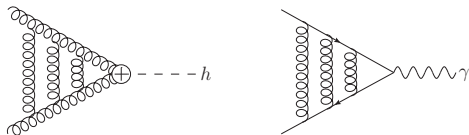


Y. Li, A. von Manteuffel, **RMS**, and H. X. Zhu, Phys. Rev. **D90** (2014) 053006



What About (Unprecedented) $\mathcal{O}(\alpha_s^4)$ Predictions?

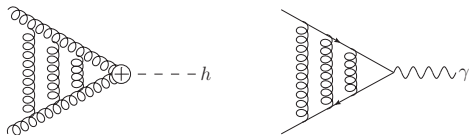
By studying the $\mathcal{O}(\alpha_s^3)$ virtual amplitudes, graphs like *e.g.*



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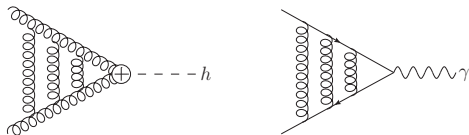


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1. At $\mathcal{O}(\alpha_s^3)$, 8 complicated basis integrals in the traditional approach; well over **100** hard(er) ones at $\mathcal{O}(\alpha_s^4)$.

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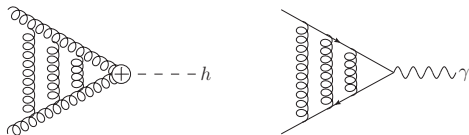


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2. Generic basis integrals at $\mathcal{O}(\alpha_s^4)$ can have, at worst, ϵ^{-8} poles; challenging to extract in an efficient way.
3. After making all ϵ poles explicit, no obvious way to evaluate the resulting convergent integrals.

Finite Integral Bases For Virtual Corrections

Andreas von Manteuffel, Erik Panzer, and **RMS**, JHEP **1502** (2015) 120;

Phys. Rev. **D93** (2016), 125014; **RMS** Phys. Rev. **D99** (2019), 105010

We proved it is always possible to pick **finite** basis integrals!



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- Finiteness can be achieved by adjusting the spacetime dimension and the denominator exponents:

$$\int \frac{d^{4-2\epsilon}k}{(p_1 - k)^2(p_2 + k)^2} \longrightarrow \int \frac{d^{6-2\epsilon}k}{[(p_1 - k)^2]^2 [(p_2 + k)^2]^2}$$



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- ▶ Fully-systematic and effective way to resolve ϵ poles.
- ▶ In many cases, a generic integration algorithm even exists!



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- ▶ Fully-systematic and effective way to resolve ϵ poles.
- ▶ In many cases, a generic integration algorithm even exists!
- ▶ I constructed first non-trivial examples of finite integrals:

$$\frac{1}{\mathcal{N}} \int \frac{d^{6-2\epsilon}k}{[(p_1 - k)^2]^2 [(p_2 + k)^2]^2} = [-(p_1 + p_2)^2]^{-1-\epsilon} \left(1 + \epsilon + 2\epsilon^2 + \dots\right)$$



Towards Virtual Higgs and Drell-Yan @ $\mathcal{O}(\alpha_s^4)$

S.-O. Moch *et. al.*, JHEP **10** (2017) 041; Phys. Lett. **B782** (2018) 627

J. M. Henn *et. al.*, JHEP **04** (2020) 018

A. von Manteuffel, E. Panzer, and **RMS**, Phys. Rev. Lett. **124** (2020), 162001

We have taken the first decisive steps towards the calculation of the virtual Drell-Yan and Higgs cross sections at $\mathcal{O}(\alpha_s^4)$!

$$\begin{aligned}\Gamma_4^r = & N_f^3 C_R \left(\frac{64}{27} \zeta_3 - \frac{32}{81} \right) + N_f^2 C_A C_R \left(-\frac{224}{15} \zeta_2^2 + \frac{2240}{27} \zeta_3 - \frac{608}{81} \zeta_2 + \frac{923}{81} \right) + N_f^2 C_F C_R \left(\frac{64}{5} \zeta_2^2 - \frac{640}{9} \zeta_3 + \frac{2392}{81} \right) \\ & + N_f C_A^2 C_R \left(\frac{2096}{9} \zeta_5 + \frac{448}{3} \zeta_3 \zeta_2 - \frac{352}{15} \zeta_2^2 - \frac{23104}{27} \zeta_3 + \frac{20320}{81} \zeta_2 - \frac{24137}{81} \right) \\ & + N_f C_A C_F C_R \left(160 \zeta_5 - 128 \zeta_3 \zeta_2 - \frac{352}{5} \zeta_2^2 + \frac{3712}{9} \zeta_3 + \frac{440}{3} \zeta_2 - \frac{34066}{81} \right) + N_f C_F^2 C_R \left(-320 \zeta_5 + \frac{592}{3} \zeta_3 + \frac{572}{9} \right) \\ & + N_f \frac{d_F^{abcd} d_R^{abcd}}{N_R} \left(-\frac{1280}{3} \zeta_5 - \frac{256}{3} \zeta_3 + 256 \zeta_2 \right) + \frac{d_A^{abcd} d_R^{abcd}}{N_R} \left(-384 \zeta_3^2 - \frac{7936}{35} \zeta_2^3 + \frac{3520}{3} \zeta_5 + \frac{128}{3} \zeta_3 - 128 \zeta_2 \right) \\ & + C_A^3 C_R \left(-16 \zeta_3^2 - \frac{20032}{105} \zeta_2^3 - \frac{3608}{9} \zeta_5 - \frac{352}{3} \zeta_3 \zeta_2 + \frac{3608}{5} \zeta_2^2 + \frac{20944}{27} \zeta_3 - \frac{88400}{81} \zeta_2 + \frac{84278}{81} \right)\end{aligned}$$

The quark and gluon cusp anomalous dimensions improve the $\mathcal{O}(\alpha_s^3)$ predictions for Higgs and Drell-Yan by allowing for full N^3 LL resummation, and we have already obtained further new analytic results for the $\mathcal{O}(\alpha_s^4)$ virtual corrections.



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Main Weakness of the Traditional Setup

Too many hard Feynman integrals are produced!



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F. Tkachov, Phys. Lett. **B100** (1981) 65; K. Chetyrkin and F. Tkachov, Nucl. Phys. **B192** (1981) 159

Integration by parts reduction to a basis of Feynman integrals



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Integration by parts reduction to a basis of Feynman integrals

- ▶ The number of Feynman diagrams gets large at $\mathcal{O}(\alpha_s^3)$ and introduces a large number of complicated integrals.
- ▶ Proceed by systematically applying Stokes's theorem to generate all possible linear relations between integrals. Subsequently, reduce to a basis set using linear algebra.
- ▶ The typical size of the linear systems at $\mathcal{O}(\alpha_s^3)$ causes problems in practice, due to **intermediate expression swell**.

S. Laporta, Int. J. Mod. Phys. **A15** (2000) 5087



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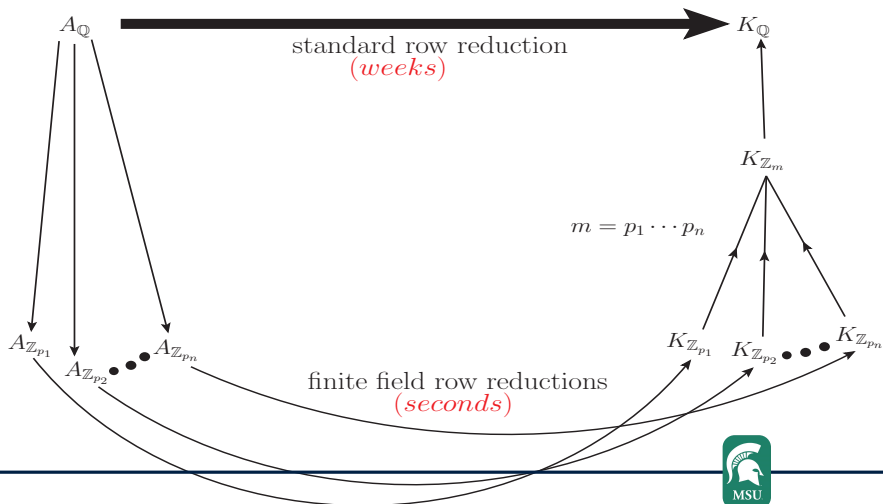
Running the best program available at the time, **Reduze 2**, took me of the order of weeks and required GBs of RAM.



Solution: Finite Fields and Rational Reconstruction

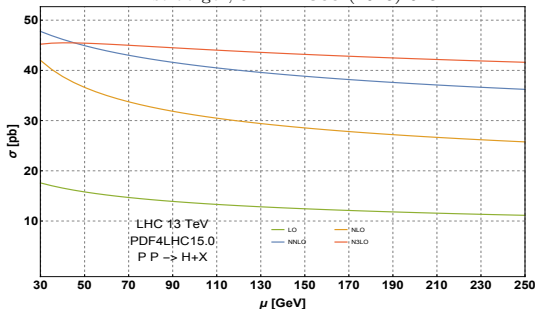
A. von Manteuffel and RMS, Phys. Lett. **B744** (2015) 101

By discussing with mathematicians, I developed a new integration by parts reduction algorithm, with polynomial run-time complexity in the size of the linear system to be solved!

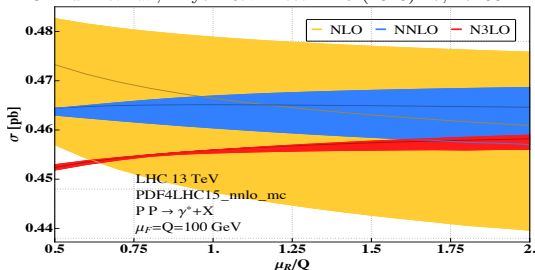


Impact: Full Higgs and Drell-Yan Predictions at $\mathcal{O}(\alpha_s^3)$

B. Mistlberger, JHEP **1805** (2018) 028



C. Duhr *et. al.*, Phys. Rev. Lett. **125** (2020) 17, 172001



My integration by parts algorithm enabled this progress!



Towards Tri-Jet Production at $\mathcal{O}(\alpha_s^2)$

$$\mathcal{M}(g(p_1)g(p_2) \rightarrow g(p_3)g(p_4)g(p_5)) = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \dots$$

$$R^{\text{NLO}} = \frac{1 + \Delta\sigma^{\text{NLO}}\alpha_s + \Delta\sigma^{\text{N}^2\text{LO}}\alpha_s^2 + \dots}{1 + \Delta\sigma^{\text{NLO}}\alpha_s + \dots} = 1 + \Delta\sigma^{\text{N}^2\text{LO}}\alpha_s^2 + \dots$$

- ▶ Once available, an important constraint on α_s .
- ▶ Depends on **5** kinematical invariants, $s_{ii+1} = (p_i + p_{i+1})^2$.
- ▶ Virtual cross section very hard, leading groups rely on **finite fields and rational reconstruction** for the integral reduction!

S. Badger *et. al.*, Phys. Rev. Lett. **123** (2019) 071601; S. Abreu *et. al.*, JHEP **1905** (2019) 084



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Machinery implemented in **FiniteFlow**, **Fire 6**, and **Kira 2!**



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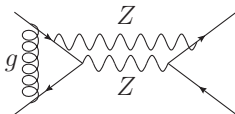
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Mixed Electroweak-QCD Drell-Yan Amplitudes

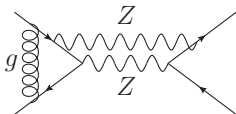


Andreas von Manteuffel and **RMS**, JHEP **1704** (2017) 129

M. Heller, A. von Manteuffel, and **RMS**, Phys. Rev. **D102** (2020), 016025

M. Heller, A. von Manteuffel, **RMS**, and Hubert Spiesberger, arXiv:2012.05918

Mixed Electroweak-QCD Drell-Yan Amplitudes



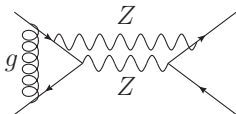
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- ▶ Besides the concrete results we obtained in terms of well-understood mathematical functions, I achieved a major conceptual breakthrough by understanding for the first time the precise relationship between **Kreimer's γ_5 scheme** and the standard **HVBM γ_5 scheme**.

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- ▶ Besides the concrete results we obtained in terms of well-understood mathematical functions, I achieved a major conceptual breakthrough by understanding for the first time the precise relationship between **Kreimer's γ_5 scheme** and the standard **HVBM γ_5 scheme**.
- ▶ Due to the fact that there are no finite counterterms required for the restoration of chiral symmetry in Kreimer's γ_5 scheme, our work suggests a **far simpler automation** of $\mathcal{O}(\alpha_s\alpha)$ or $\mathcal{O}(\alpha^2)$ Feynman diagram calculations!

How Does This Work at the Practical Level?



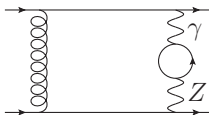
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- ▶ At each order in perturbation theory, I envisaged to generate the Standard Model diagrams of interest with `QGraf` and then pipe them through `Reduze 2` in order to match them onto suitable integral families.



How Does This Work at the Practical Level?

- ▶ At each order in perturbation theory, I envisaged to generate the Standard Model diagrams of interest with **QGraf** and then pipe them through **Reduze 2** in order to match them onto suitable integral families.
- ▶ To accommodate the general case, I modified **Reduze 2**, adding my own fully-general **C++** routine to partial fraction power products of propagator denominators with the same momentum but different masses, *e.g.* $(k^2 - m_z^2)^{-1}(k^2)^{-1}$:



High-Performance Computing



High-Performance Computing

- ▶ Performed numerator algebra in `Mathematica` for $\sim 50,000$ multi-loop diagrams for projects using high-performance computing clusters available at JGU and MSU.



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- ▶ At various times, needed to do scripting in `Bash` and become familiar with scheduling in both `LSF` and `Slurm`.
- ▶ Despite the infinite licenses available at many research institutions, `Mathematica` is closed-source, so it is reasonable to wonder whether it makes sense to employ it.



Dealing With Mathematica Bugs

Turn a setback into an opportunity to improve the code!



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- ▶ In Mathematica v10.3.1, `Apart[# , x1] &` would fail on “complicated” inputs such as:

$$\frac{x_2(d x_1 + t)^3((x_1 + t)x_2 + x_2^2(x_1 + d + x_1^2))^2}{x_3(t x_1 + (x_2 + x_3 + 1))^4((-s x_3)x_1 - t x_2)^5(x_3 + x_2 + x_1 x_2)^3}$$



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- ▶ With a little effort, I was able to generalize the approach to univariate partial fractioning discussed by Erik Panzer in his thesis and arrive at an implementation far superior to the one available in even the latest version of Mathematica.



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- ▶ In Mathematica v10.3.1, `Apart[# , x1]` & would fail on “complicated” inputs such as:

$$\frac{x_2(d x_1 + t)^3((x_1 + t)x_2 + x_2^2(x_1 + d + x_1^2))^2}{x_3(t x_1 + (x_2 + x_3 + 1))^4((-s x_3)x_1 - t x_2)^5(x_3 + x_2 + x_1 x_2)^3}$$

- ▶ With a little effort, I was able to generalize the approach to univariate partial fractioning discussed by Erik Panzer in his thesis and arrive at an implementation far superior to the one available in even the latest version of Mathematica.
- ▶ Principally, this was possible by making a more intelligent choice about how to organize the output; in v12.0.0, the output of `Apart` has a `ByteCount` of 3613880, whereas my replacement has a `ByteCount` of only 660776.





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- ▶ Will eventually cover `Spark`, `SQL`, `TensorFlow`, and details of the most widely-used machine learning techniques.
- ▶ Besides the well-known applications of machine learning to particle physics phenomenology, I would like to see if I can develop a custom scheduler to serve the pheno group's high-performance computing needs in an optimal way.

The Big Picture

Fundamental Large Hadron Collider Processes

Efficient Computer Algebra for Multi-Loop Calculations

Computing, Scientific Software, and Machine Learning

Summary



The Bottom Line

- ▶ Groundbreaking work on fundamental LHC processes requires new techniques and dedicated effort.
- ▶ First *ab initio* analytic calculation of the cusp anomalous dimensions and first analytic calculation of the collinear anomalous dimensions done; finite parts of four-loop quark and gluon form factors calculable in current setup with known methods and modest computing resources.
- ▶ Important conceptual and technical progress on EW-QCD Drell-Yan; virtual cross sections now within reach.
- ▶ Massively-parallel integration by parts algorithm I pioneered applicable to many hard calculations of current interest. In fact, for most processes discussed in this talk, no other methods have produced comparable results.
- ▶ Machine learning algorithms will become ever more important to particle physics. Exciting to see what is next!

