Computing amplitudes in QFT

Challenges in precision calculations

Jonathan Ronca

Workshop sul Calcolo nell'INFN

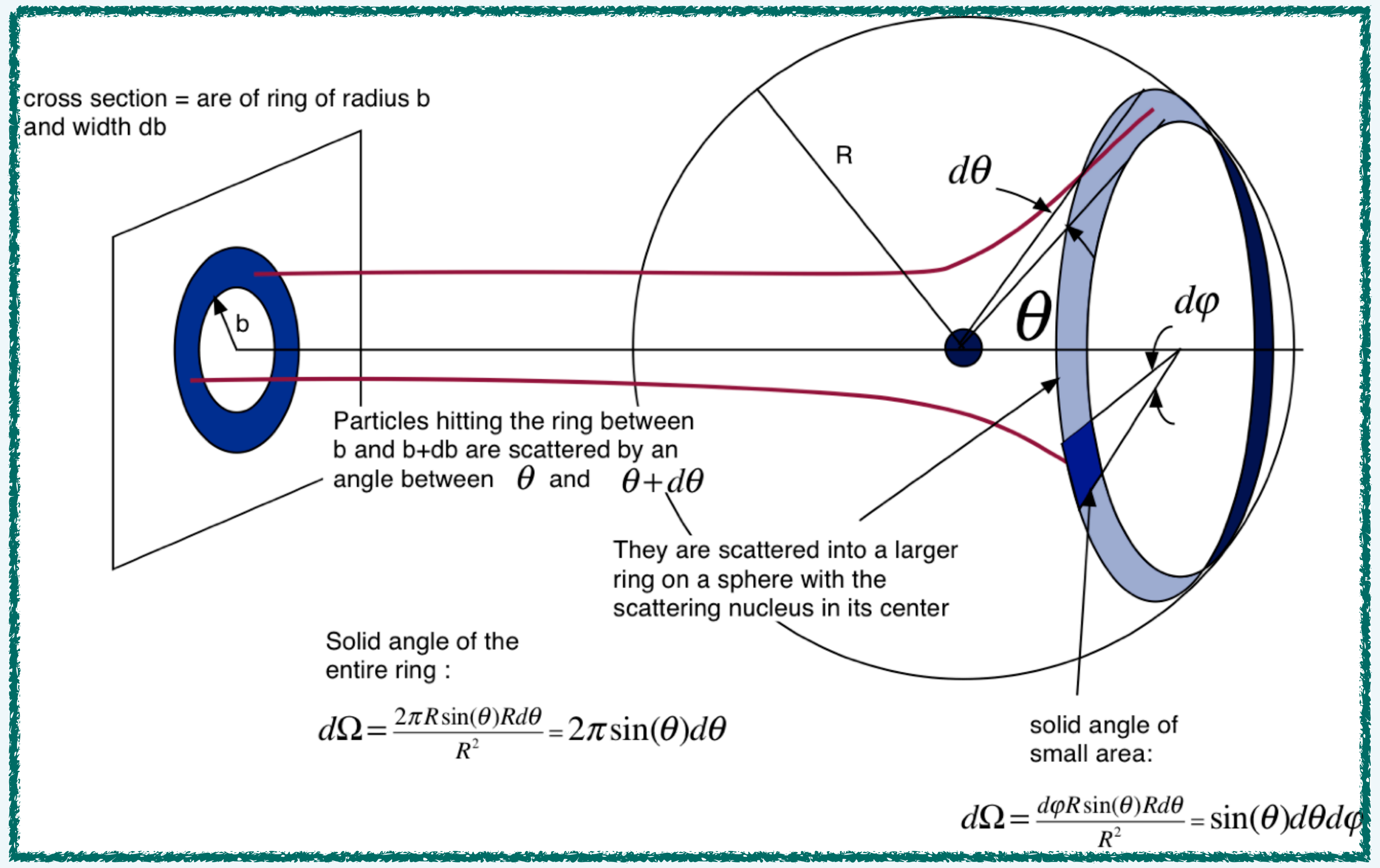
La Biodola - Isola d'Elba
26-30 Maggio 2025

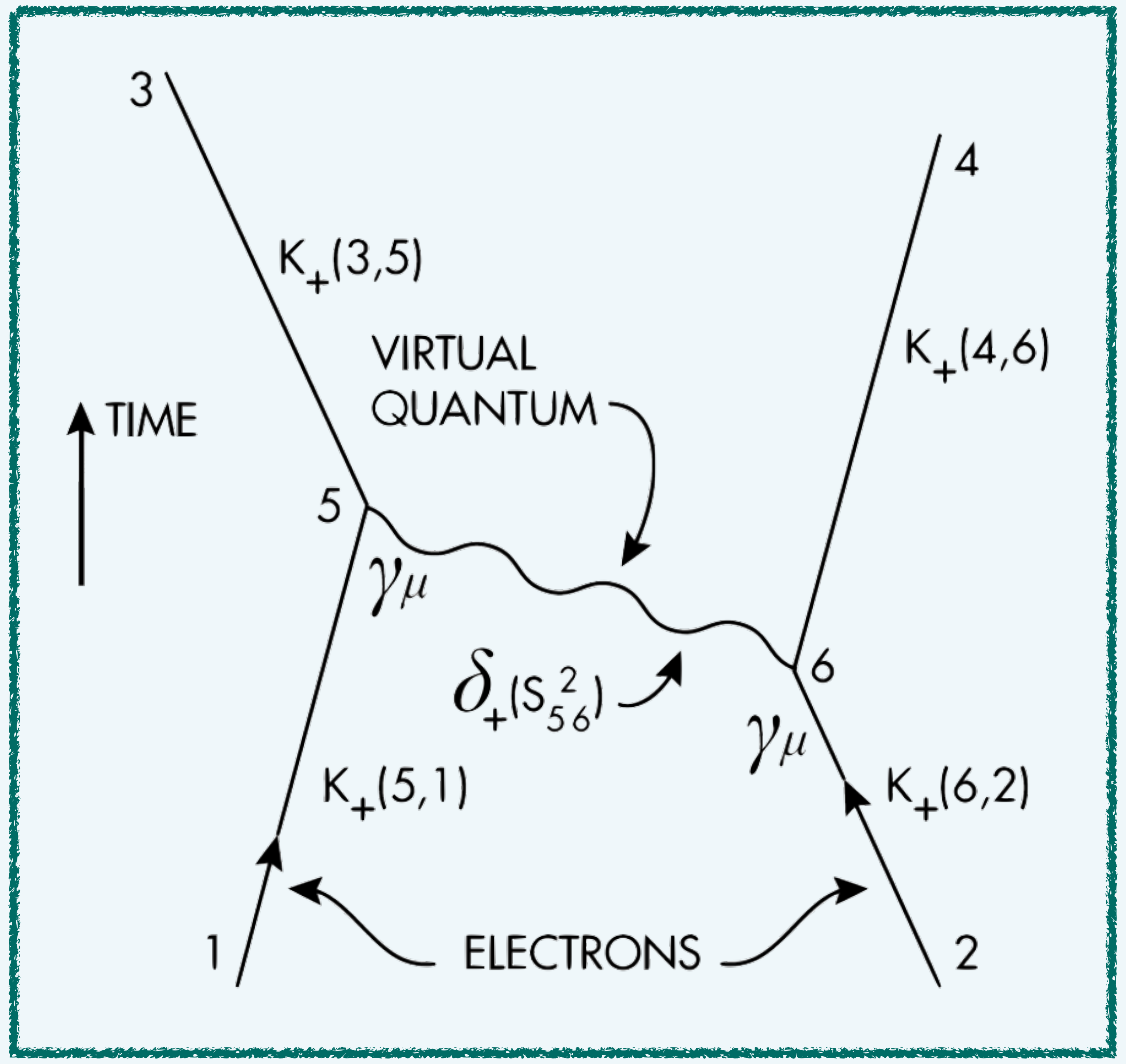
Dipartimento di Fisica e Astronomia Galileo Galilei

INFN PADOVA
Istituto Nazionale di Fisica Nucleare
Sezione di Padova

26 May 2025

Introduction



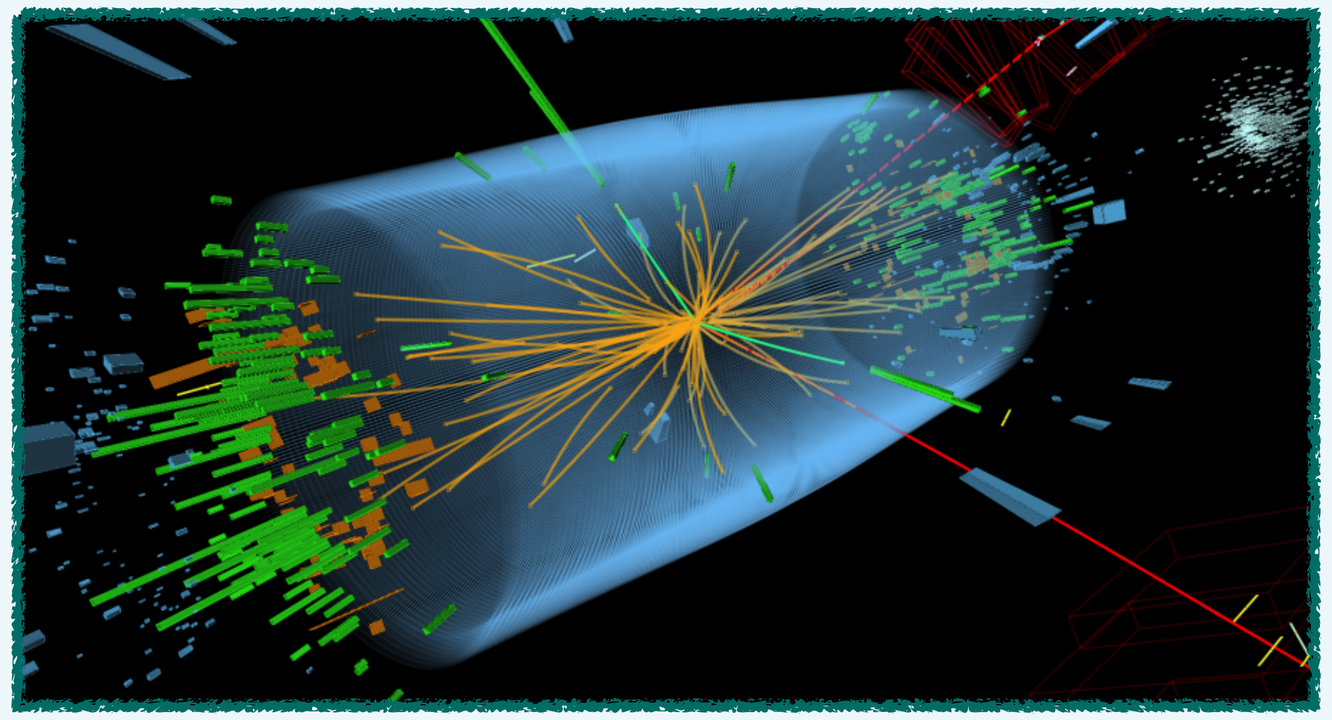


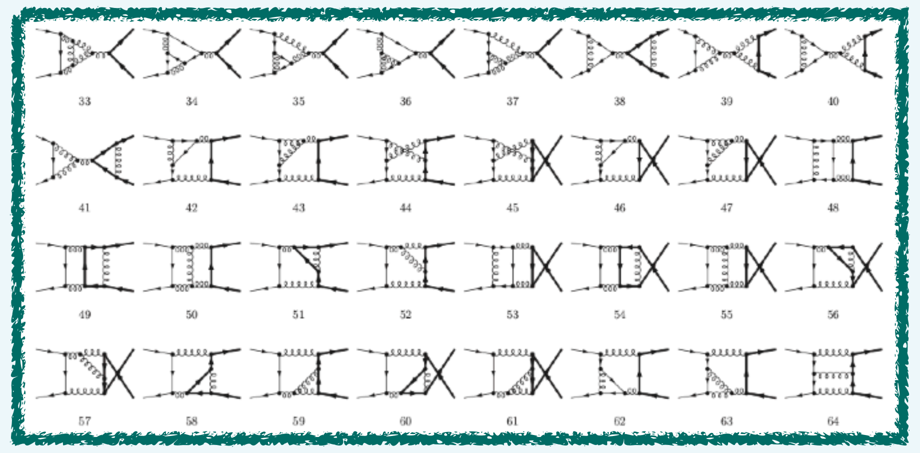
[Feynman (1950)]

- Scattering processes are an ubiquitous phenomena in Nature
- Quantitative way to describe interactions
- Interdisciplinary topic: Physics, Mathematics, Computer Science…
- Link between several fields in physics

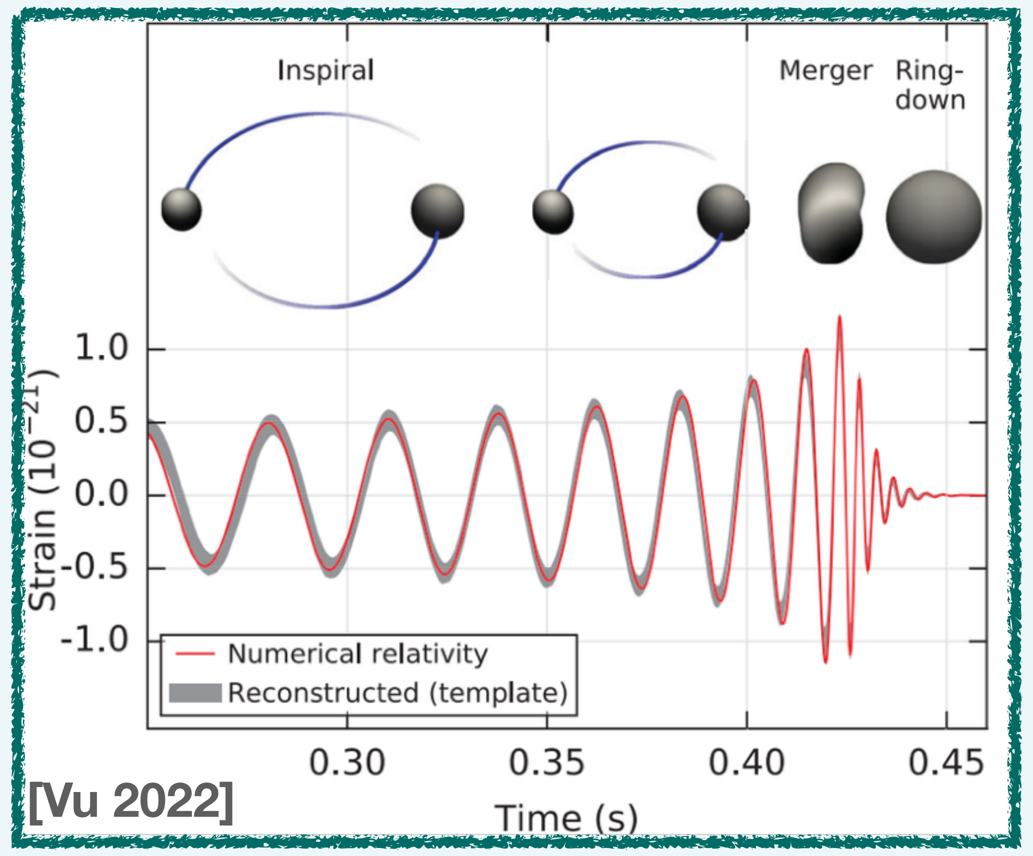
Introduction

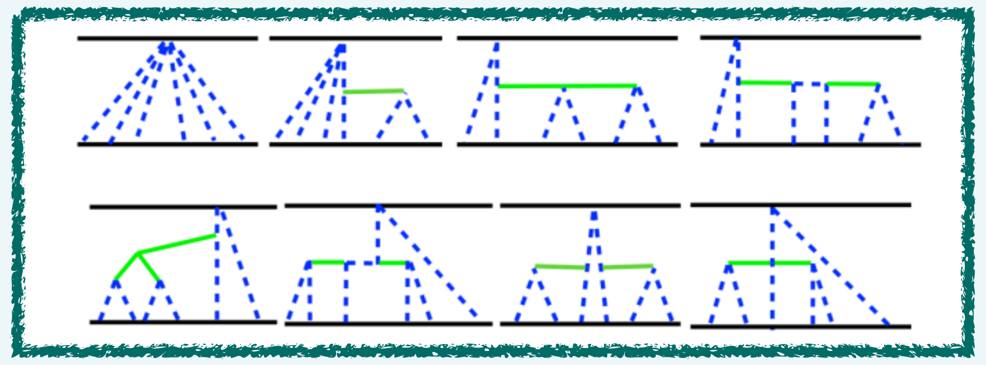
Collider physics



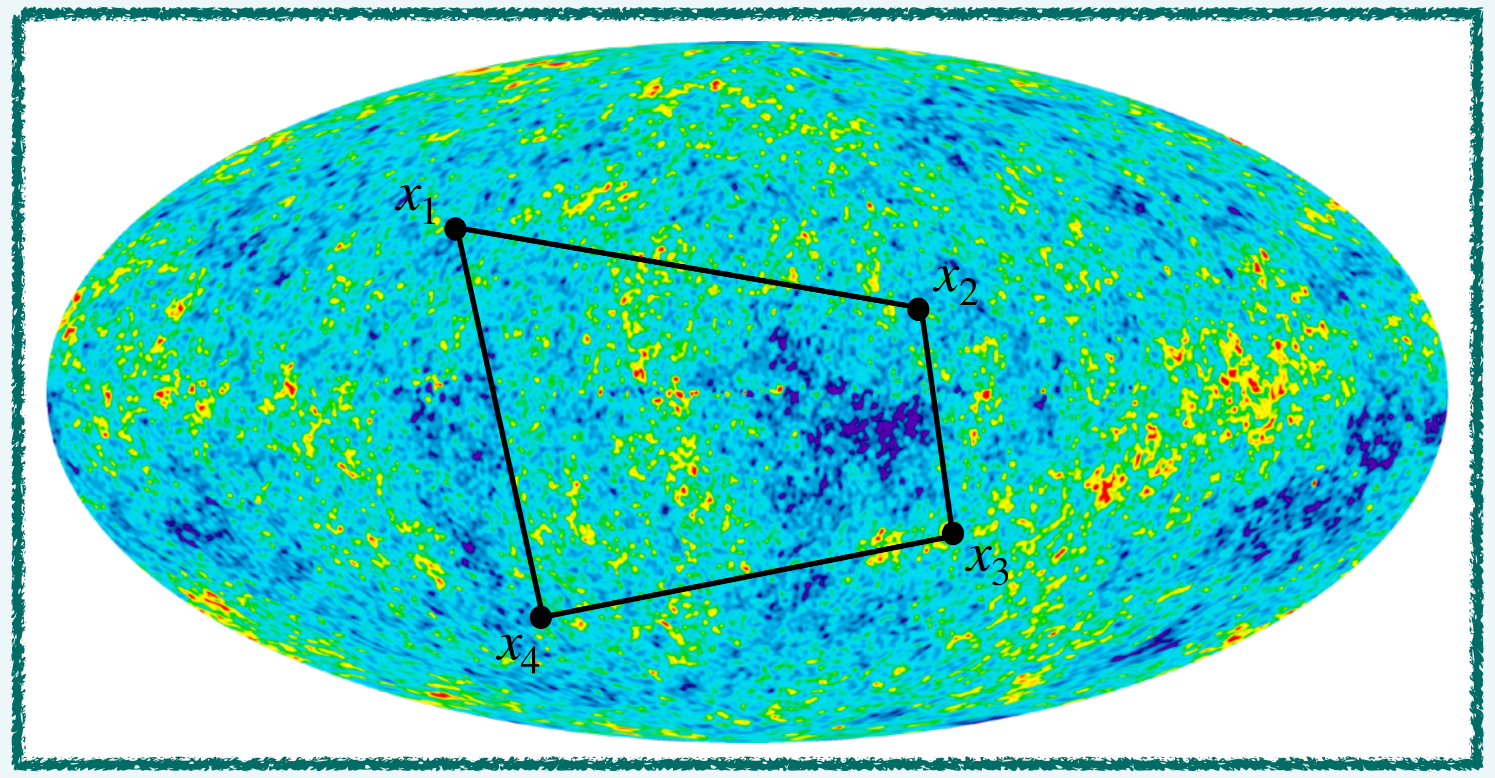


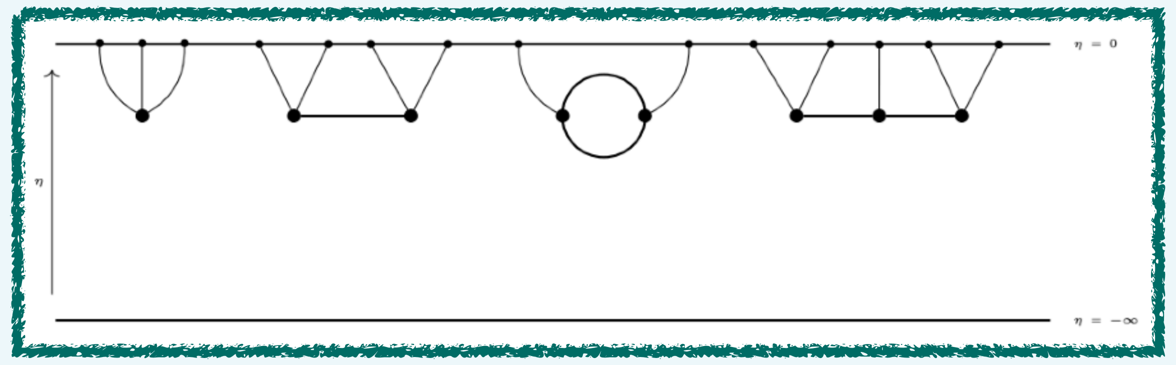
Classical General Relativity





Cosmology





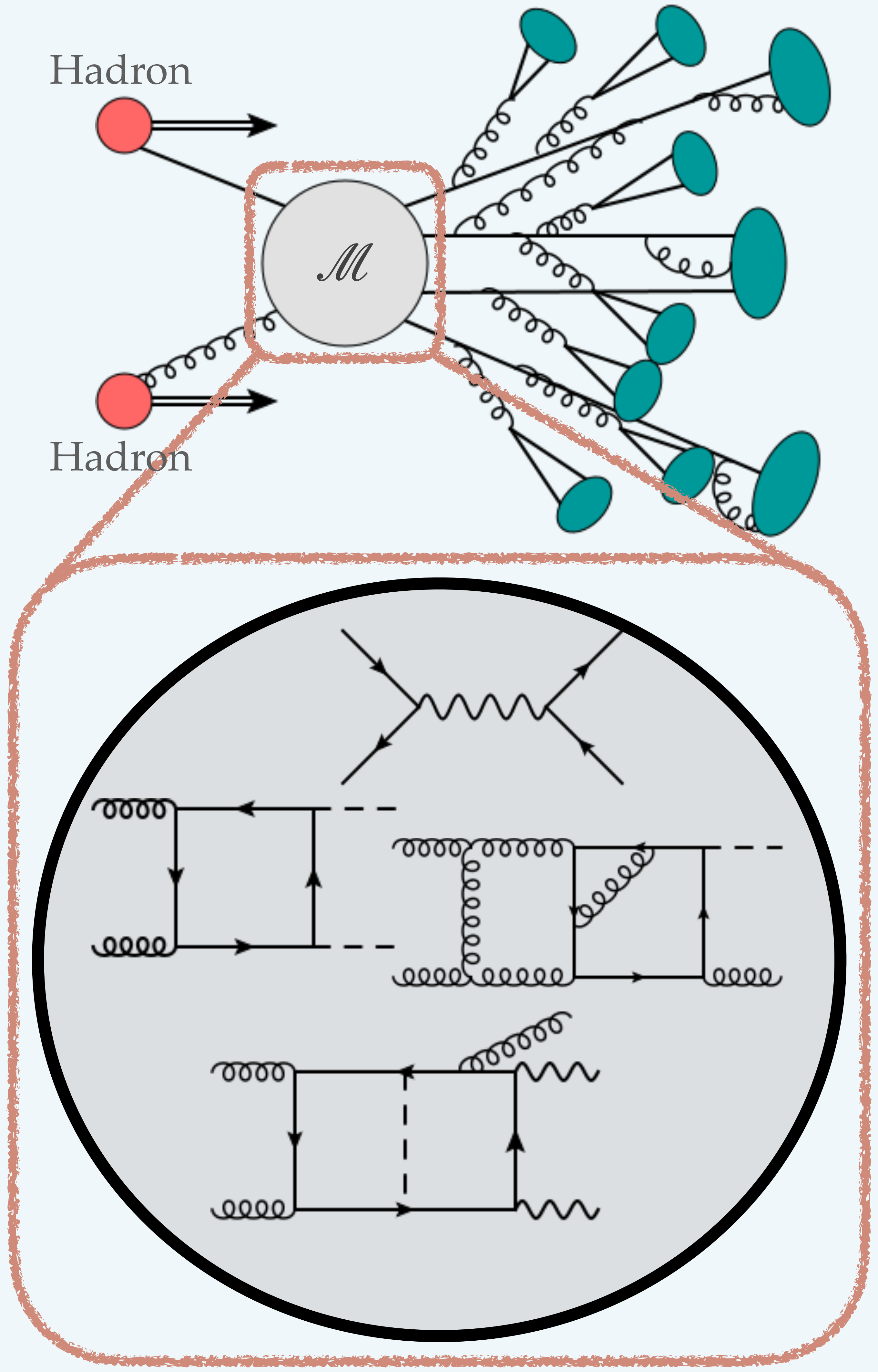
Definition. *Physics is a part of mathematics devoted to the calculation of integrals of the form* $\int g(x)e^{f(x)}dx$. *Different branches of physics are distinguished by the range of the variable* x *and by the names used for* $f(x)$, $g(x)$ *and for the integral.* [...]

Of course this is a joke, physics is not a part of mathematics. However, it is true that the main mathematical problem of physics is the calculation of integrals of the form

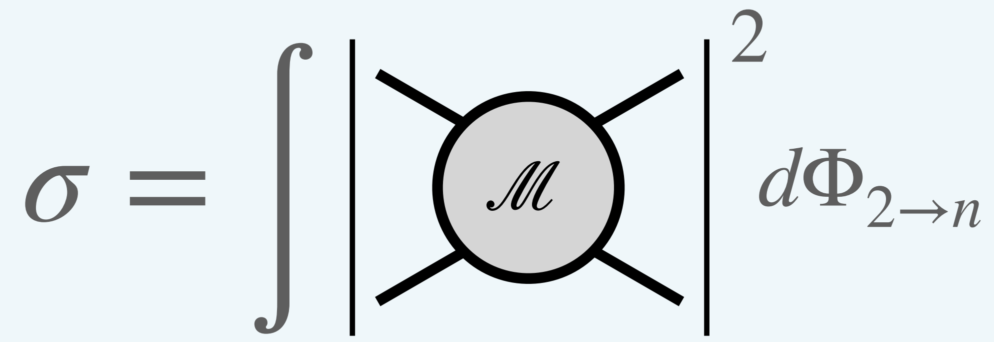
$$I(g) = \int g(x)e^{-f(x)}dx$$

[Schwarz, Shapiro (2018)]

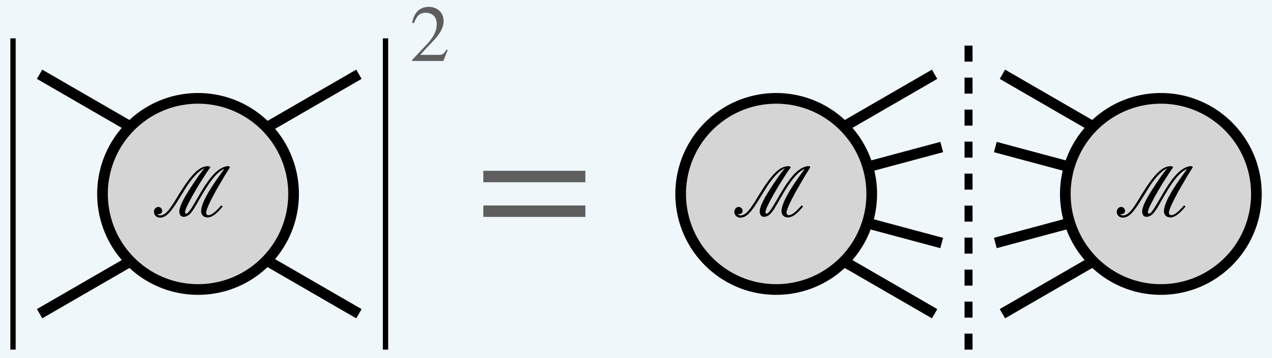
Scattering Amplitudes: Basics



Observables related to a quantum probability density



Probability density

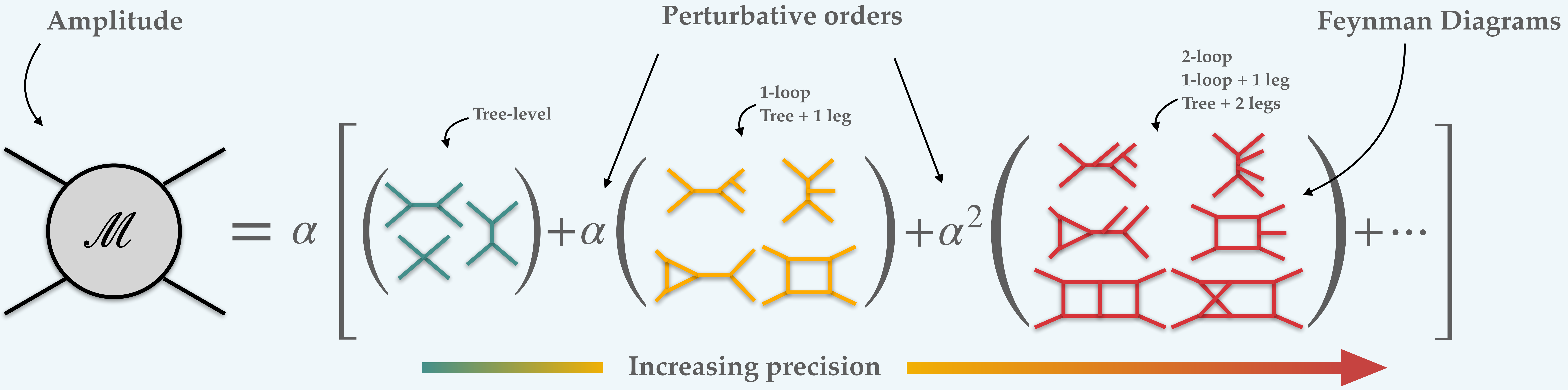


Integrating density via Monte Carlo methods

- Event generators
- Energy distributions
- Angular distributions
- Grids

Needs for fast numerical evaluations

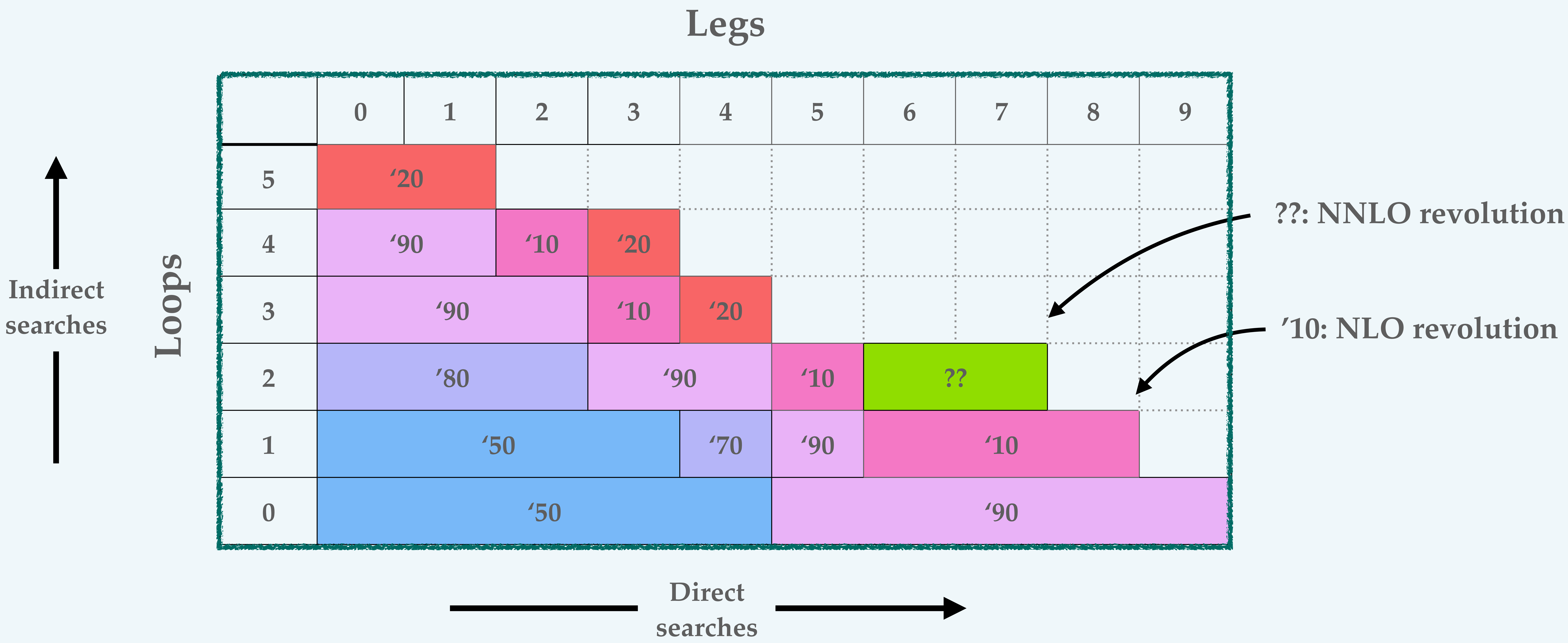
Scattering Amplitudes: Perturbative expansion



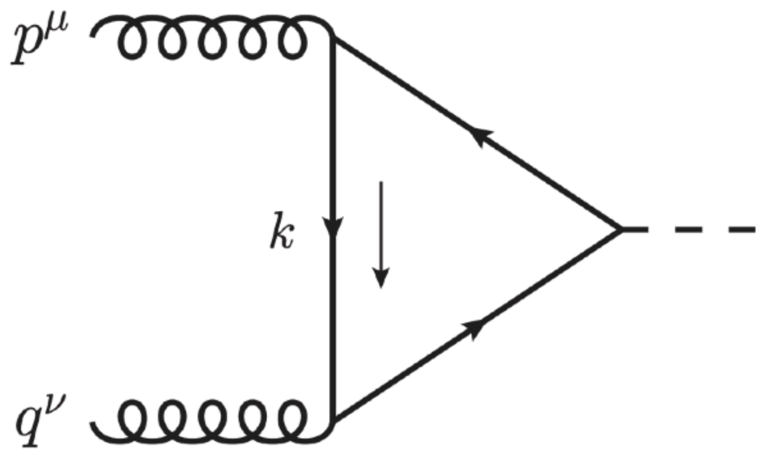
Precision increases with the higher perturbative orders:

- **More precision**:
  - **More loops** → numbers of integrations
  - **More legs** → more variables
- **Complexity grows quickly** (graph combinatorics involved)
- Complicated analytic structures (poles, branch cuts…)

Computing amplitudes

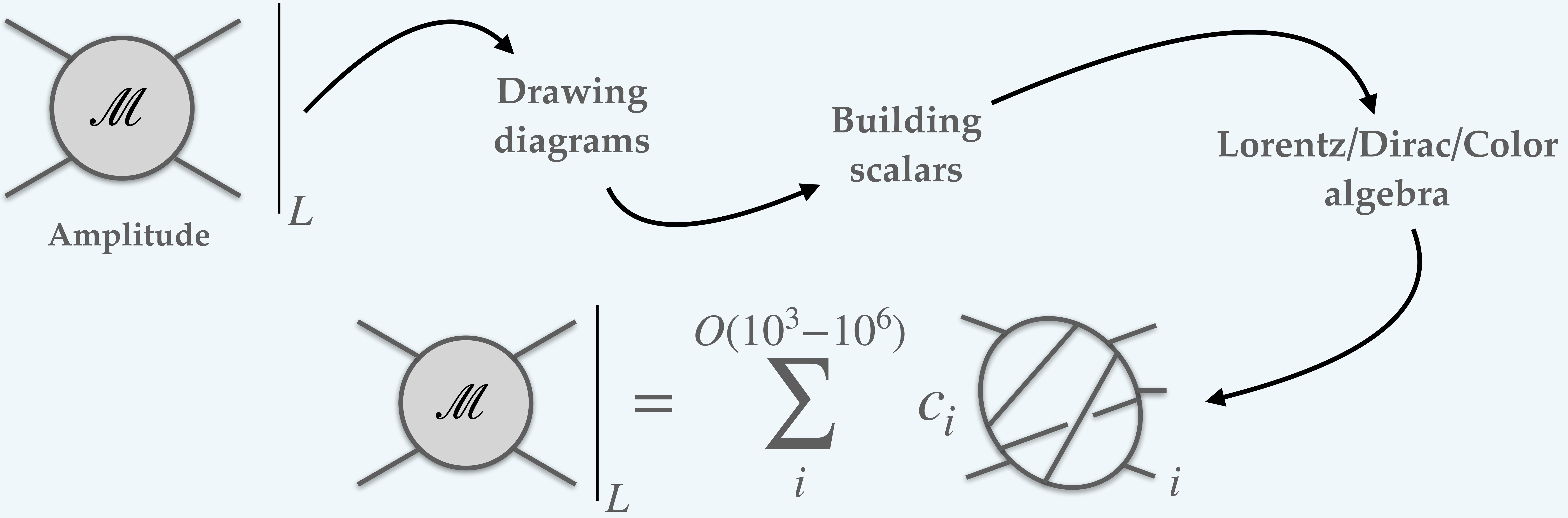


Computing amplitudes: Feynman Integrals

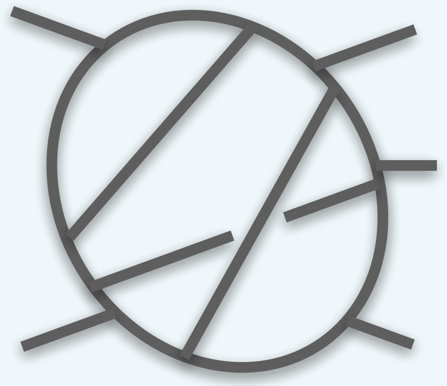


$$= (-)(2)\frac{i}{(4\pi)^2}(4\pi\mu^2)^{2-\frac{d}{2}}\int_k \mathrm{Tr}\left[(-ig_s\gamma_\mu T^a)\frac{i(\not{k}-\not{p}+m_t)}{(k-p)^2-m_t^2}\left(-i\frac{m_t}{v}Y_j\right)\frac{i(\not{k}+\not{q}+m_t)}{(k+q)^2-m_t^2}(-ig_s\gamma_\nu T^b)\frac{i(\not{k}+m_t)}{k^2-m_t^2}\right]$$

Computing amplitudes: Feynman Integrals



Feynman Integrals



$$= \int \left(\prod_{i=1}^{L} d^d k_i \right) \frac{1}{D_1^{a_1} \cdots D_n^{a_n}} = I_{a_1,\ldots,a_n}(d; \bar{x})$$

Feynman integrals are the core of an amplitude:

- D_i are (usually) linear or quadratic functions of k_i's
- Space-time **dimension** d is kept as a **variable**
- $\bar{x}$ are the **scales** of the process (i.e. external legs + internal states)
- Very few cases where a primitive can be found
- We are interested in an **expansion** around $d = 4$

Computing amplitudes: Feynman Integrals

Nowadays experimental precision requires:

- Theoretical precision of the **per-mille level**
- **2nd** and **3rd perturbative order** amplitudes
- Diagrammatically:
  - 2- and 3- loop amplitudes
  - 4 and 5 external legs
  - >5 kinematical variables and parameters
- Theoretical precision $\Longleftrightarrow$ **efficient loop computations**

n	2	3	4	5	6	7	8
# of diagrams	4	25	220	2485	34300	559405	10525900

Tree-level!

Table 1: The number of Feynman diagrams contributing to the scattering process $gg \to$ n g .

[Mangano, Parke (1990)]

Large symbolical expression:

- $O(10^3)$ diagrams for 2- and 3- loop amplitudes
- **Multivariate polynomials**
- Typically subexpressions of $O(10^2)$ MBytes
- Cutting-edge amplitudes of $O(10)$ GBytes

Public codes:

- QGraf
- FeynArts
- FeynCalc
- LoopIn
- AIDA
- Tapir
- MadGraph

[Bigazzi,Mandal,Mastrolia,Torres Bobadilla (WIP)]

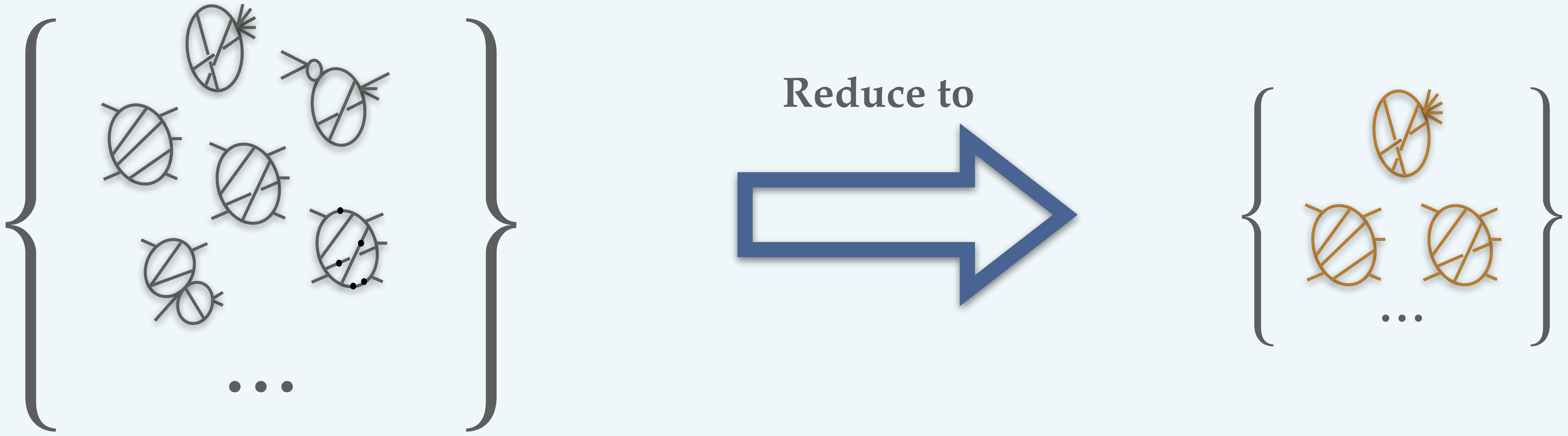
Need for fast evaluations:

- Key-element for **physical observables**
- Included in **Monte Carlo integrators**
- Employed in **phenomenological studies**

Languages:

- Mathematica
- FORM
- Symbolica
- Python
- Fortran
- C/C++

Computing Integrals: Reduction

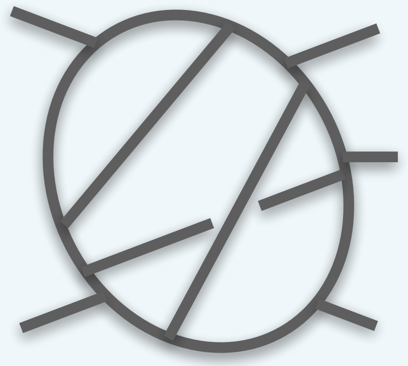


Many: $O(10^6)$

Few: $O(10^2)$

Computing Integrals: Reduction

Integration-by-parts identities (IBPs)

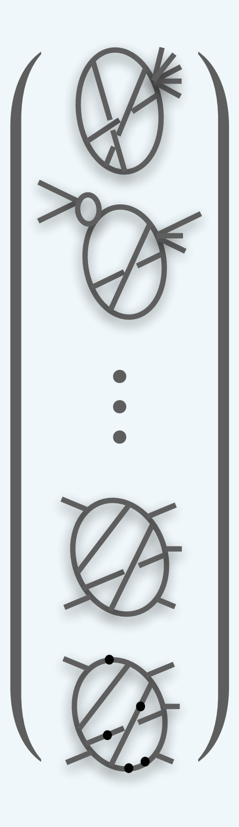
O_{ij}  $= 0$

Seed operator

Rational functions of $\bar{x}, d$

Needed integrals

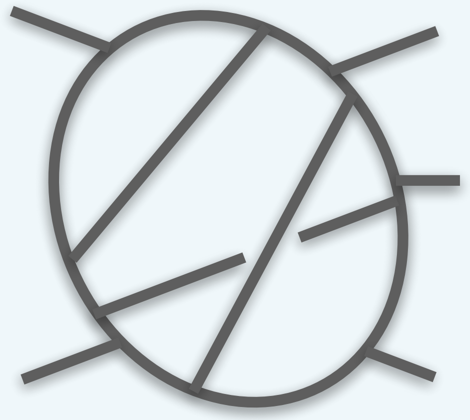
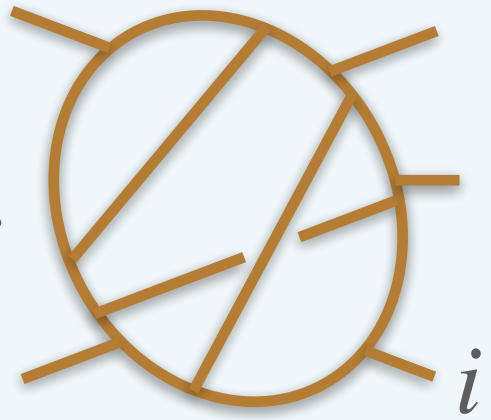
Generated identities

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & & a_{1M} \\ a_{21} & a_{22} & \cdots & & a_{2M} \\ & & \ddots & & \\ \vdots & \vdots & & \ddots & \\ a_{N1} & a_{N2} & & & a_{NM} \end{pmatrix}$$  $= 0$

Algorithm:

- Lots of **linearly dependent** rows
- **Gauss elimination**
- IBPs system rank $\ll$ #equations
- Choice of independent integrals: **Master Integrals**
- Back-substitution $\Longrightarrow$ integral relations

Reduction to Master Integrals

 $= \sum_{i}^{O(10^2)} c_i$  $_i$

Computing Integrals: Reduction

Very large sparse system of equations:

- $O(10^6) - O(10^8)$ equations for 3-loop amplitudes
- **Symbolic** solutions of IBP system
- **Finite field reconstruction** methods
- GPU support

Smart choices of "seed" integrals reduces the # equations:

- Syzygy equations
- Block triangular form
- Improved seedings
- ML and Genetic Algorithms

Alternative methods:

- Adaptive Integrand Reduction
- Intersection theory
- Groebner basis

Public Codes:

- Reduze
- Air
- Kira
- FIRE
- Rational Tracer
- FinRed
- Rational Tracer
- FiniteFlow
- LiteRed
- Blade
- NeatIBPs

CAS:

- Mathematica
- GiNaC
- Fermat
- Singular
- Firefly
- Flint
- Symbolica
- Maple

Computing Integrals: Reduction

It is very time-consuming process. For cutting-edge calculation:

- $\mathcal{O}(1)$ **month** of running time, even on clusters
- $\mathcal{O}(10)$ **GBytes** of identities
- Dramatically **increasing the size** of the amplitudes
- **Rational reconstruction** methods need **lot** of RAM
- 16GB RAM/CPU appears to be an ideal ratio
- $\mathcal{O}(1)$ TByte RAM required for **Mathematica** packages

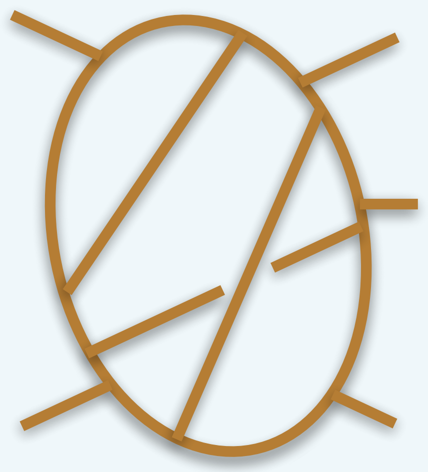
	`Kira 2.3`	`Kira dev`	`Kira dev` + RATRACER
# of generated equations	16 872 564	76 045	-
# of selected equations	1 157 381	41 998	-
# of terms	23 053 485	734 833	-
Time to generate and select	1 259 s	14 s	-
Memory to generate and select	30 GiB	1.9 GiB	-
Probe time	38 s	1.2 s	0.12 s

[Lange,Usovitsch,Wu (2024)]

Technical issues:

- Batch systems usually settled with cap wall time of $\mathcal{O}$(day)
- Special need for **queues** with **longer runtime** allowed, like $\mathcal{O}$(month)
- Public codes have only few checkpoints
- **Checkpoints** are ofter **not reliable**

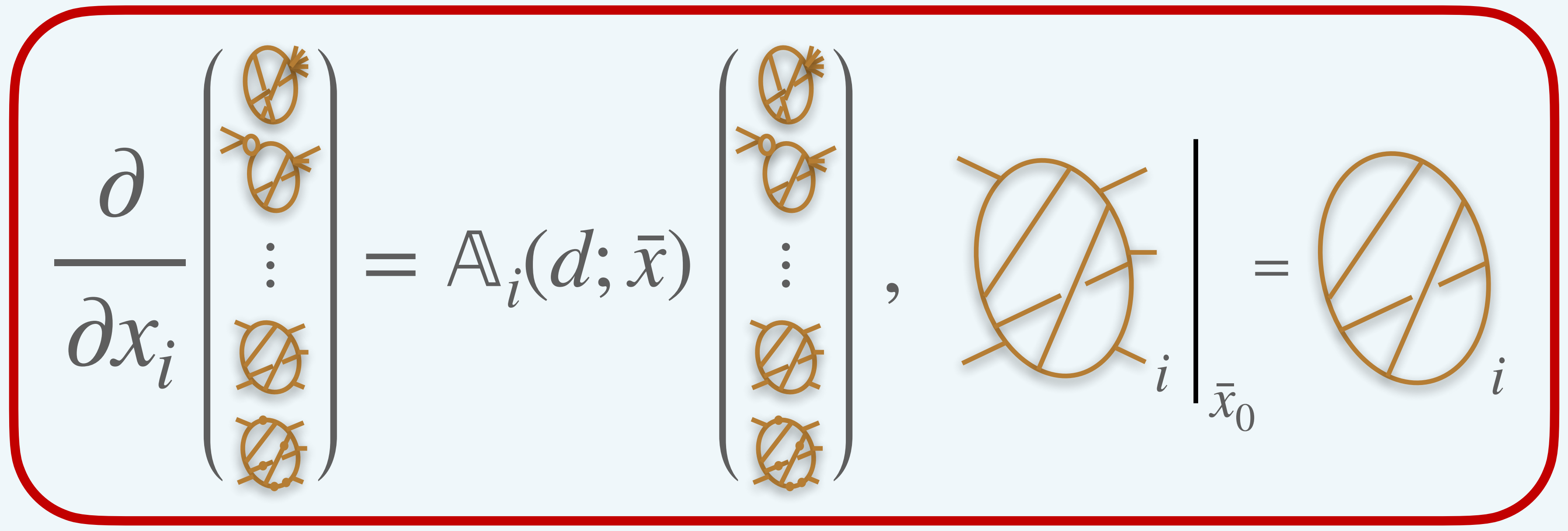
Computing Integrals: Evaluation

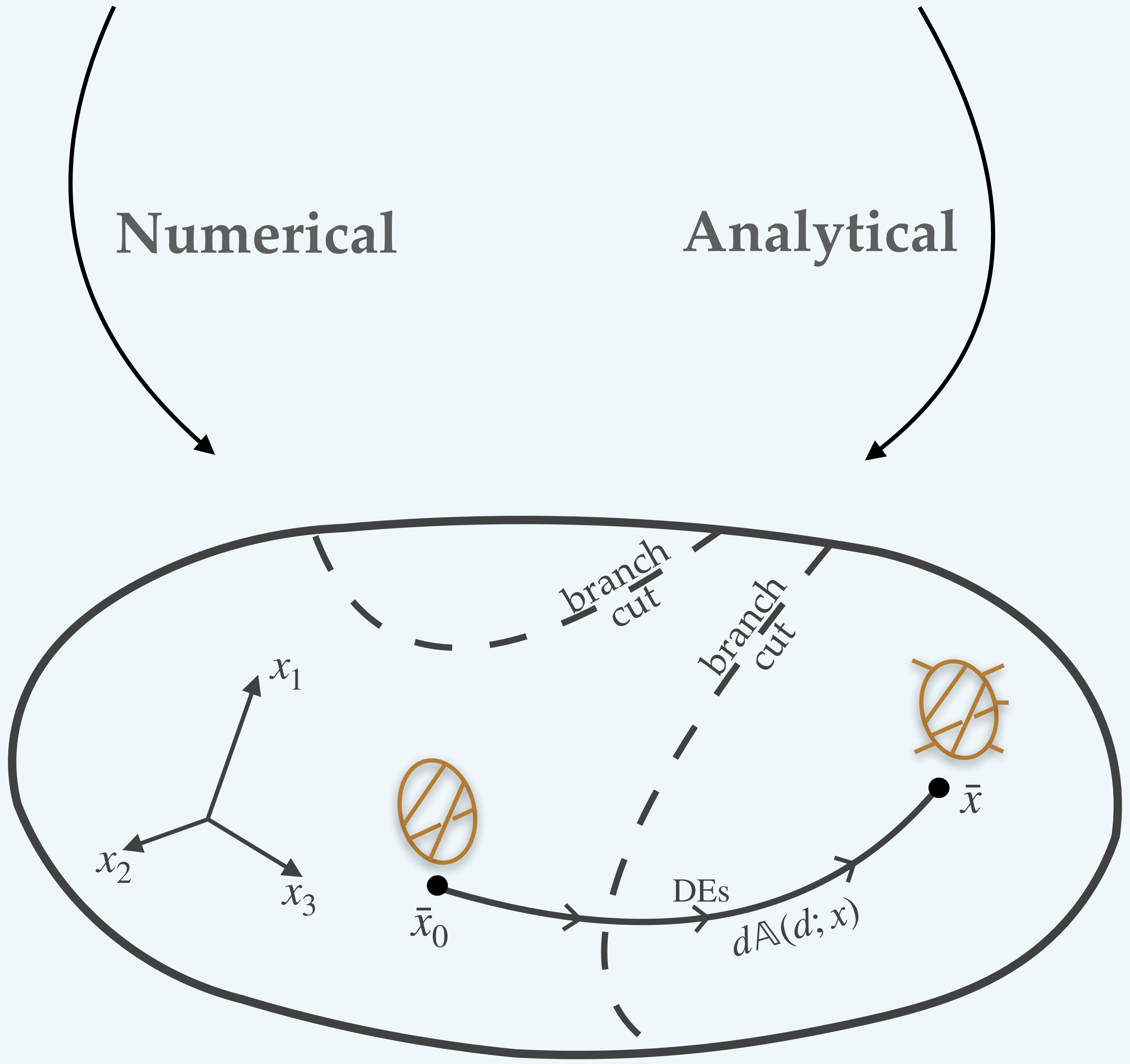


$$\left(x_1 = val_1, x_2 = val_2, \ldots\right) \quad = \quad ?$$

Computing Integrals: Evaluation

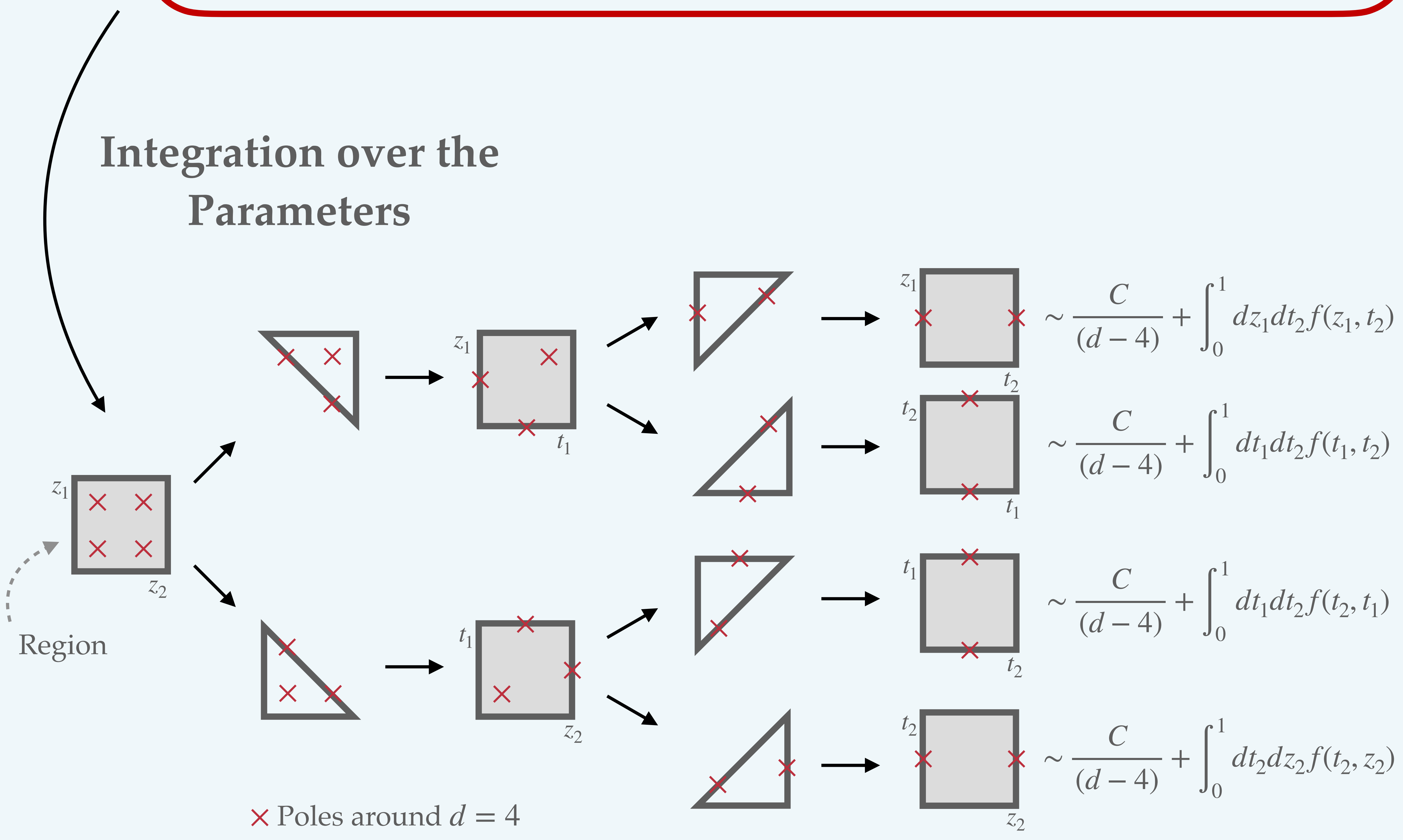
Differential Equations





Integral representations

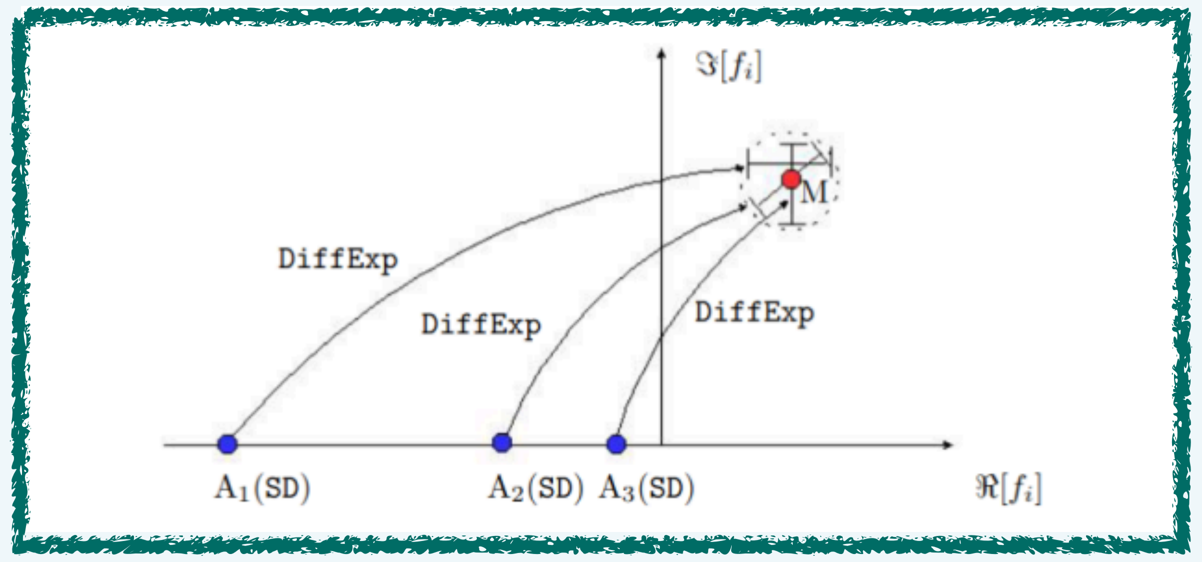
$$= I_{a_1,\ldots,a_n}(d;\bar{x}) \propto \int_{\mathscr{C}} \left(\prod_j \frac{dz_j}{z_j} z_j^{a_j}\right) \frac{\mathscr{U}(\bar{z})^{\sum a_i-(L+1)\frac{d}{2}}}{\mathscr{F}(\bar{x},\bar{z})^{\sum a_i-L\frac{d}{2}}}$$



Computing Integrals: Evaluation

Evaluating Feynman Integrals is non-trivial:

- 2- and 3- loop amplitudes described by $O(10^2)$ Master Integrals
- **Curse of dimensionality**: $O(10)$ integration variables
- Convoluted **integration regions**: branch cuts, poles…
- **Slow** Monte Carlo convergence
- Analytical integration often **not possible**
- Non-trivial symbolical manipulations:
  - Analytical continuation
  - Frobenius method
  - Fuchsian form
  - …



[Dubovyk,Freitas,Gluza,Grzanka,Hidding,Usovitsch (2022)]

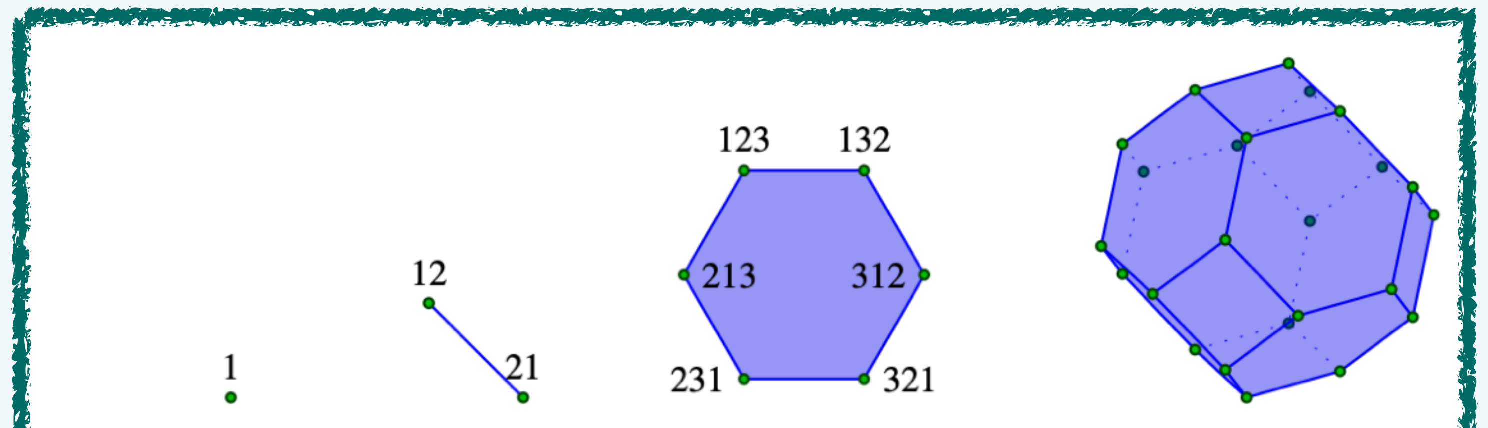


Figure 1: The first four permutohedra where it is easily seen from the explicit vertex coordinates (permutations) that all edges are parallel to $\mathbf{e}_i - \mathbf{e}_j$ for $i \neq j$.

[Borinsky,Munch,Tellander (2023)]

Current investigations:

- Analytical solution:
  - **dlog representation**
  - classifying **function spaces**
  - Ansatz for **letters**
- Efficient **numerical solution of DEs** for Feynman Integrals
- **Improving** Monte Carlo **sampling**

Public Codes:

- SecDec
- pySecDec
- FeynTrop
- FIESTA
- Lotty
- HandyG
- DiffExp
- SeaSyde
- PolyLogTools
- AMFlow
- LINE

Languages:

- Python
- Mathematica
- C/C++

Computing Integrals: Evaluation

Numerical evaluation of Feynman Integrals:

- Many codes for solving DEs are written in **Mathematica**
- **Not-suitable for clusters**
- **Licenses** issues
- Recent development: C implementation LINE

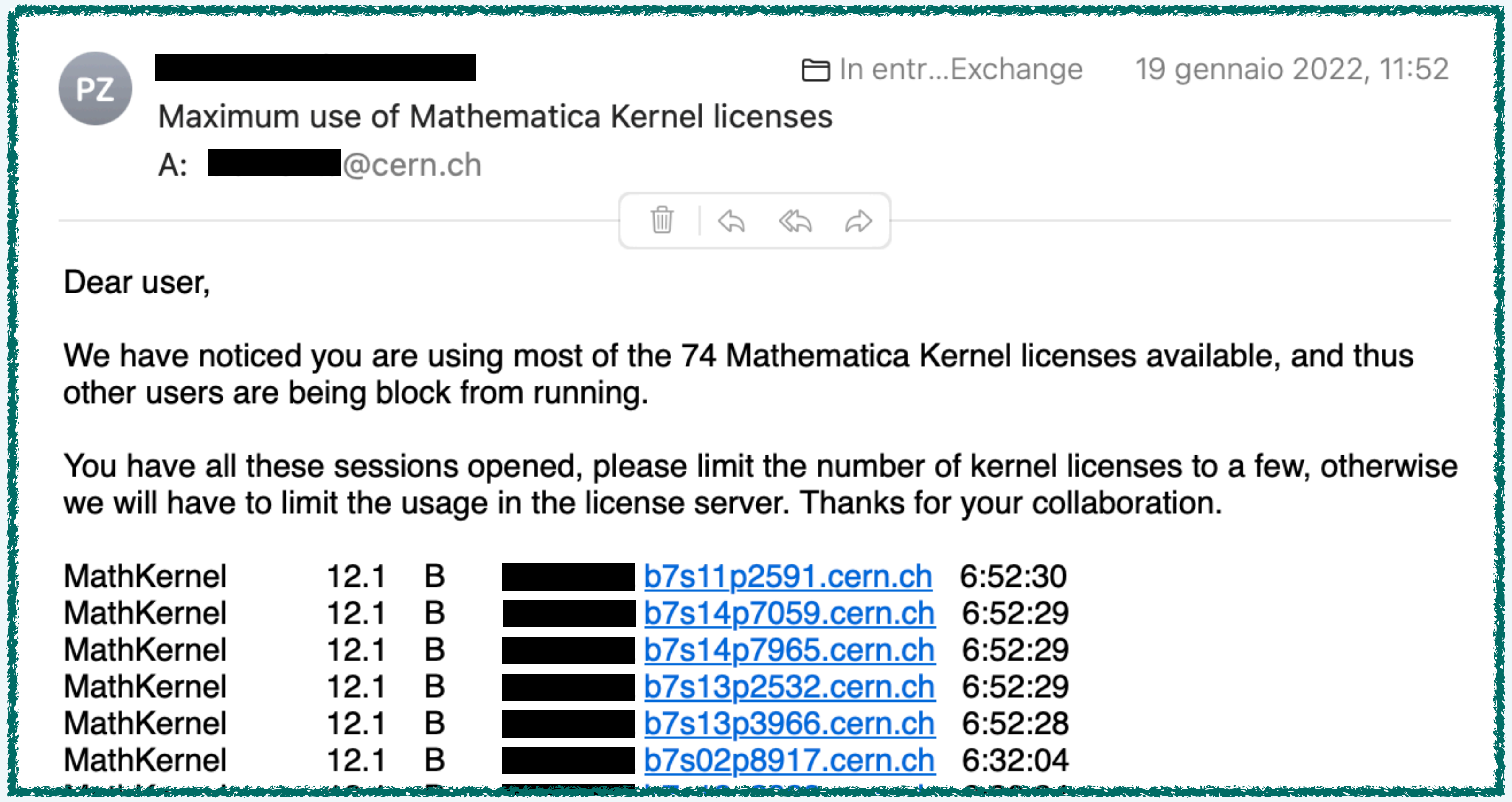
[Prisco,JR,Tramontano (2025)]

Typical running time (2- or more- loop integrals)

- O(minute) to O(day)
- **prohibitive** time for **on-the-fly** evaluations
- Better suited for **grids** production

Improving the methods

- Better **MIs basis choice**
- Numerical evaluation of **iterated integrals**
- Getting **insights** from other research fields?



PZ [redacted] In entr...Exchange 19 gennaio 2022, 11:52

Maximum use of Mathematica Kernel licenses

A: [redacted]@cern.ch

Dear user,

We have noticed you are using most of the 74 Mathematica Kernel licenses available, and thus other users are being block from running.

You have all these sessions opened, please limit the number of kernel licenses to a few, otherwise we will have to limit the usage in the license server. Thanks for your collaboration.

MathKernel	12.1	B	[redacted]	b7s11p2591.cern.ch	6:52:30
MathKernel	12.1	B	[redacted]	b7s14p7059.cern.ch	6:52:29
MathKernel	12.1	B	[redacted]	b7s14p7965.cern.ch	6:52:29
MathKernel	12.1	B	[redacted]	b7s13p2532.cern.ch	6:52:29
MathKernel	12.1	B	[redacted]	b7s13p3966.cern.ch	6:52:28
MathKernel	12.1	B	[redacted]	b7s02p8917.cern.ch	6:32:04

[Colleague (2022)]

Flagship Use Case [UC2.1.3]

Usecase HPC.spoke2.WP1 /ADVANCED CALCULUS FOR PRECISION PHYSICS

Nodes: UNIBO - UNICAL - UNIMIB - UNIPD

- **Five research directions:**
  - **1. Models & Diagrams**
  - **2. Amplitudes & Integrals**
  - **3. Cross Sections & Events**
  - **4. Physics at Colliders**
  - **5. Beyond Colliders**

The software developed in this research program will have a major impact on Collider Phenomenology, as well as on Cosmology and Mathematics.

- Standard Model Physics
- Beyond Standard Model Physics
- Parton Distributions Functions
- Higgs boson and Heavy Particles Physics
- Effective Field Theories for Quantum and Classical Physics
- Scattering Amplitudes
- Physics of the Universe and Gravitational Waves Physics
- Computational Algebraic Geometry

[Mastrolia (2024)]

Flagship Use Case [UC2.1.3]

Motivation

Flagship Use Cases [UC2.1.3] : Advanced Calculus for Precision Physics

LOOPIN
Loop Integrals

A completely automated code for numerical evaluation of Scattering Amplitude

What we are aiming for LoopIn to be?

- Mathematica front-end (user-friendly)
- Minimal number of inputs
- From the generation of the amplitude to its numerical evaluation
- Modular: LoopIn has to be able to be interfaced with any code
- Flexible: User can manipulate the IO of LoopIn (with care)
- Every module of LoopIn will produce its own output
- Parallelizable
- Designed for any number of loop

[JR (2024)]

Conclusions

Current precision frontier requires

- Observables predictions at **per-mille level**
- 2- and 3- loop, 4+ legs amplitudes
- Being able to evaluate amplitudes efficiently

Amplitude as active field of research

- **Mathematical** understanding of Feynman Integrals
- **Physics** insights on amplitudes structure
- More **general integrands** can be treated with these techniques:
  - Fourier integrals
  - Generalized unitarity
- Study of **function spaces**
- **Bootstrapping** methods
- Help from algebraic geometry, cohomology…

On the computational side:

Heavy and time-consuming processes

- Need for **high-ratio** RAM/CPU
- **Special queues** with very large wall time

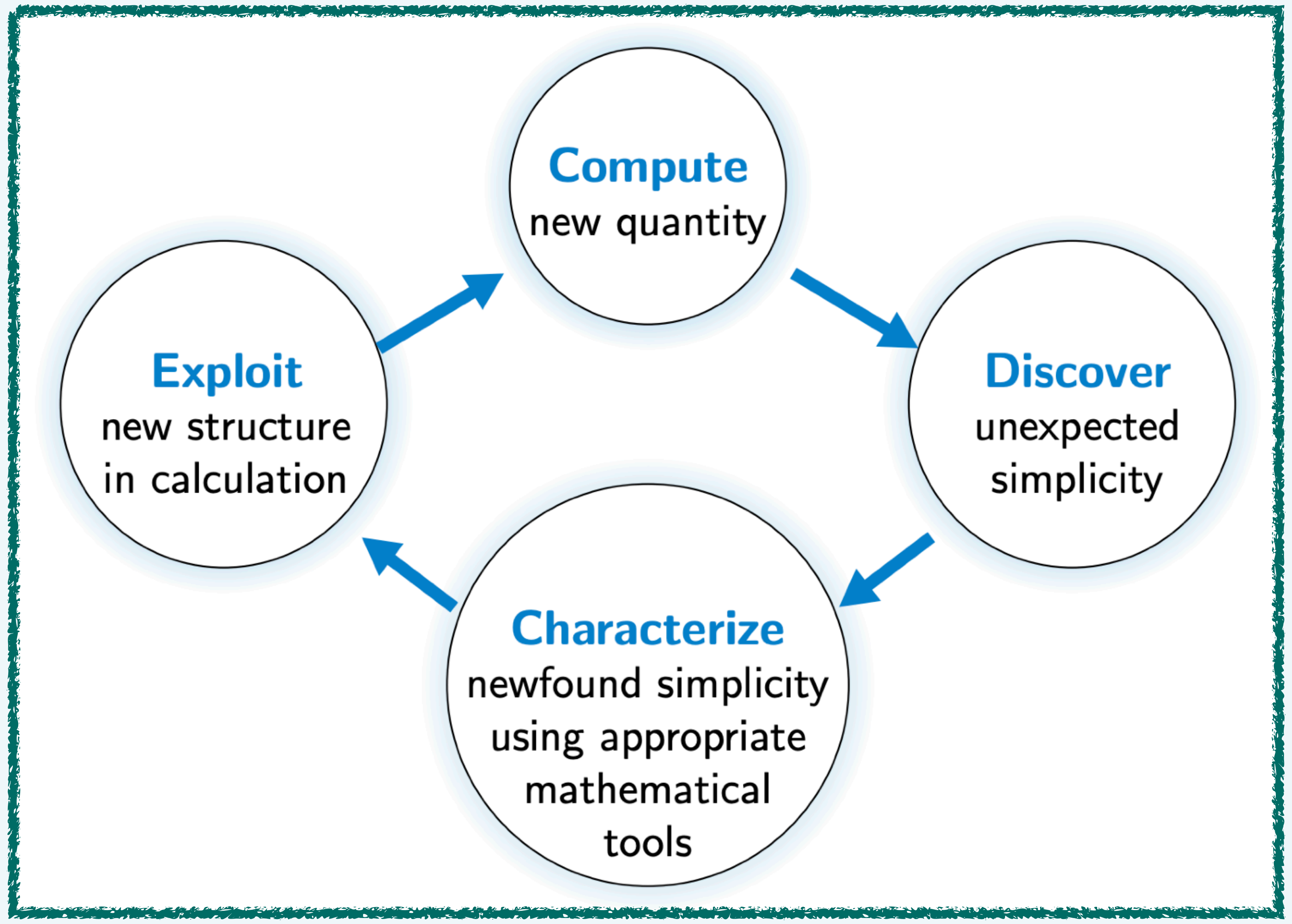
Many codes for our community are written in Mathematica

- Non-educational institutions have **limited amount of licenses**
- Using university (**educational**) licenses?

Codes are mostly written by PhDs and post-docs

- Their **maintenance** usually **ends** together with their contract
- Possibility of **IT task/position** devoted to code **optimization/maintenance**?

The Virtuous circle



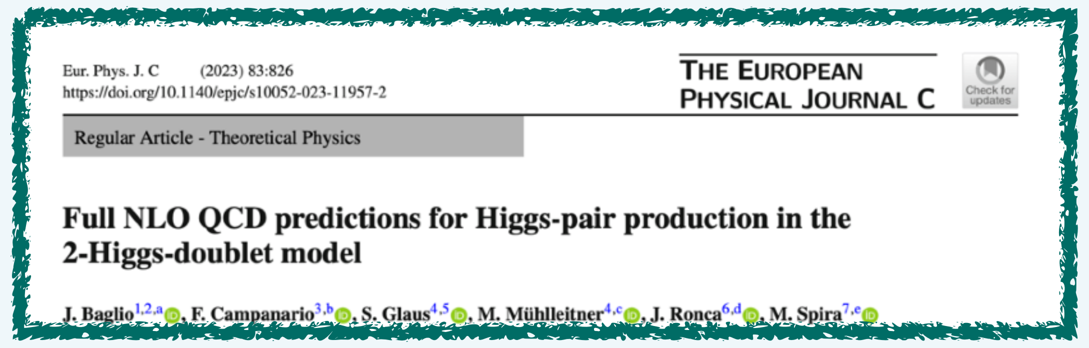
[McLeod (2024)]

“The very advanced counting system used by elementary particle theorists for counting the loops is: ‘One, two, many,’”

— Ettore Remiddi

Thank you for your attention!

Backup: $gg \to HH$ cross section



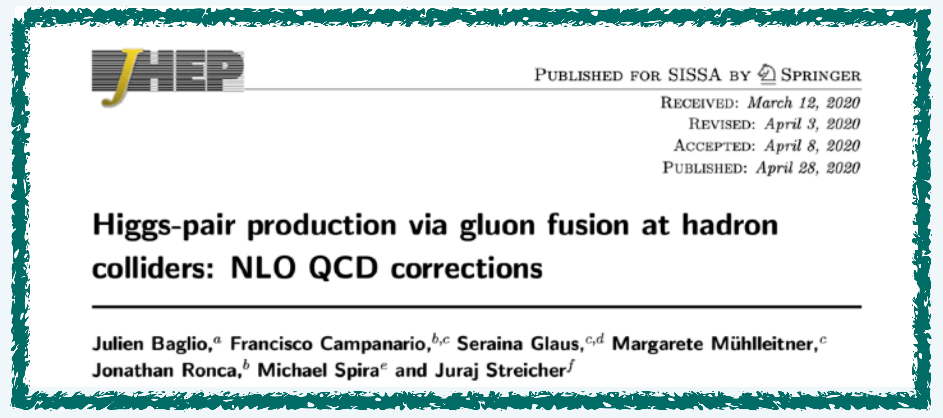
Eur. Phys. J. C (2023) 83:826
https://doi.org/10.1140/epjc/s10052-023-11957-2

THE EUROPEAN PHYSICAL JOURNAL C

Regular Article - Theoretical Physics

Full NLO QCD predictions for Higgs-pair production in the 2-Higgs-doublet model

J. Baglio[1,2,a], F. Campanario[3,b], S. Glaus[4,5], M. Mühlleitner[4,c], J. Ronca[6,d], M. Spira[7,e]



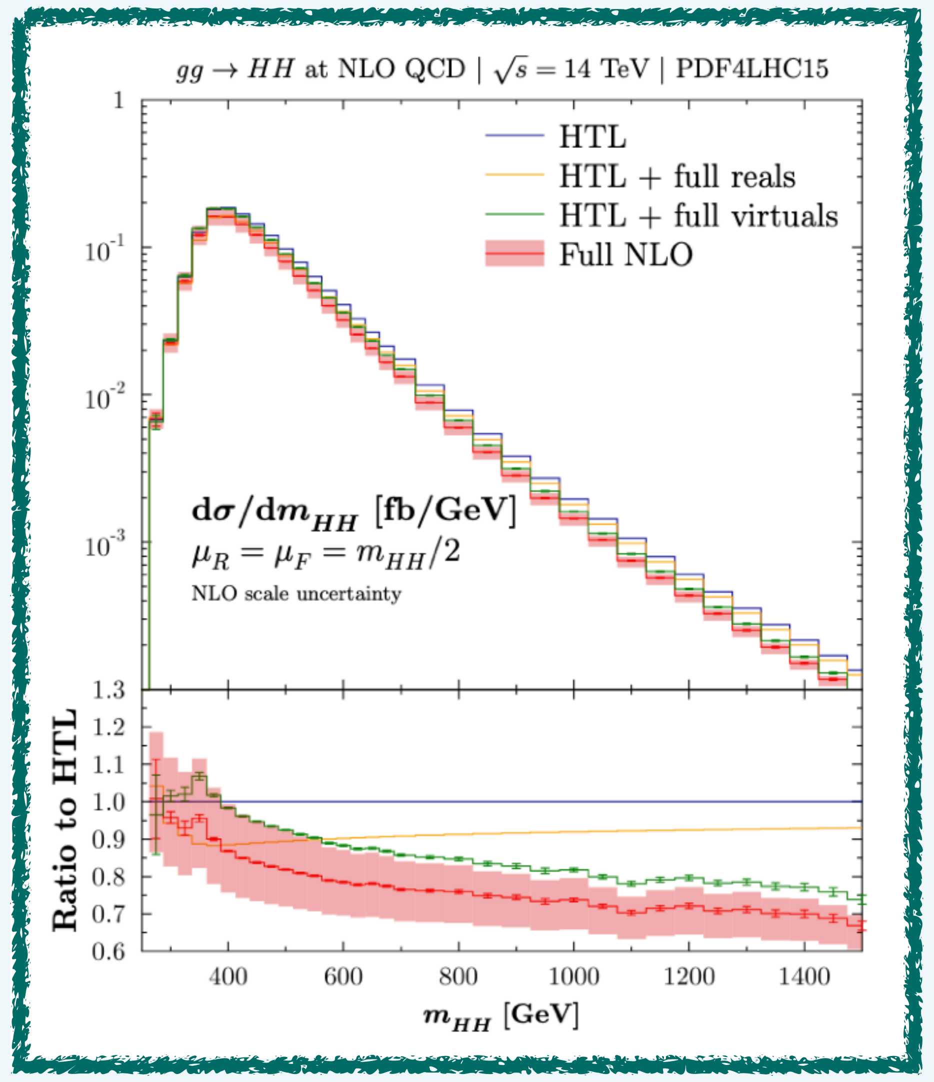
JHEP

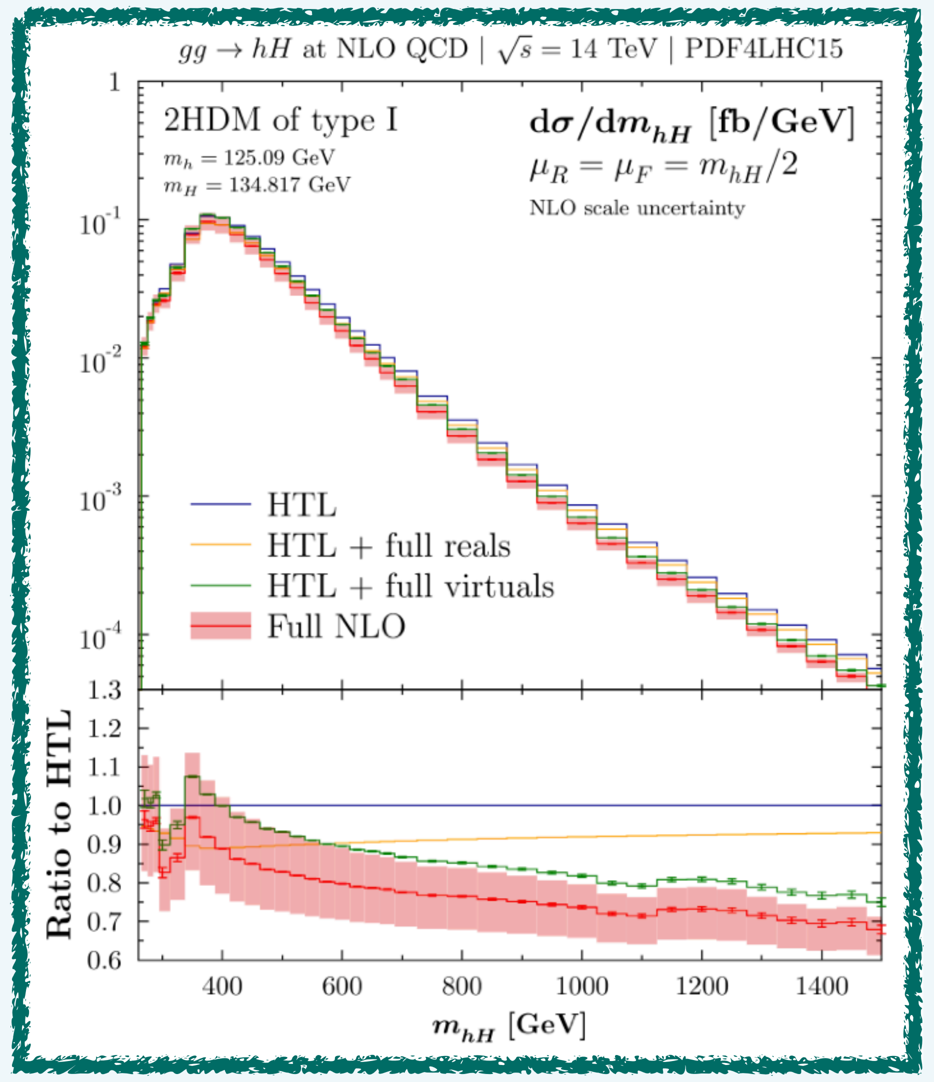
PUBLISHED FOR SISSA BY SPRINGER

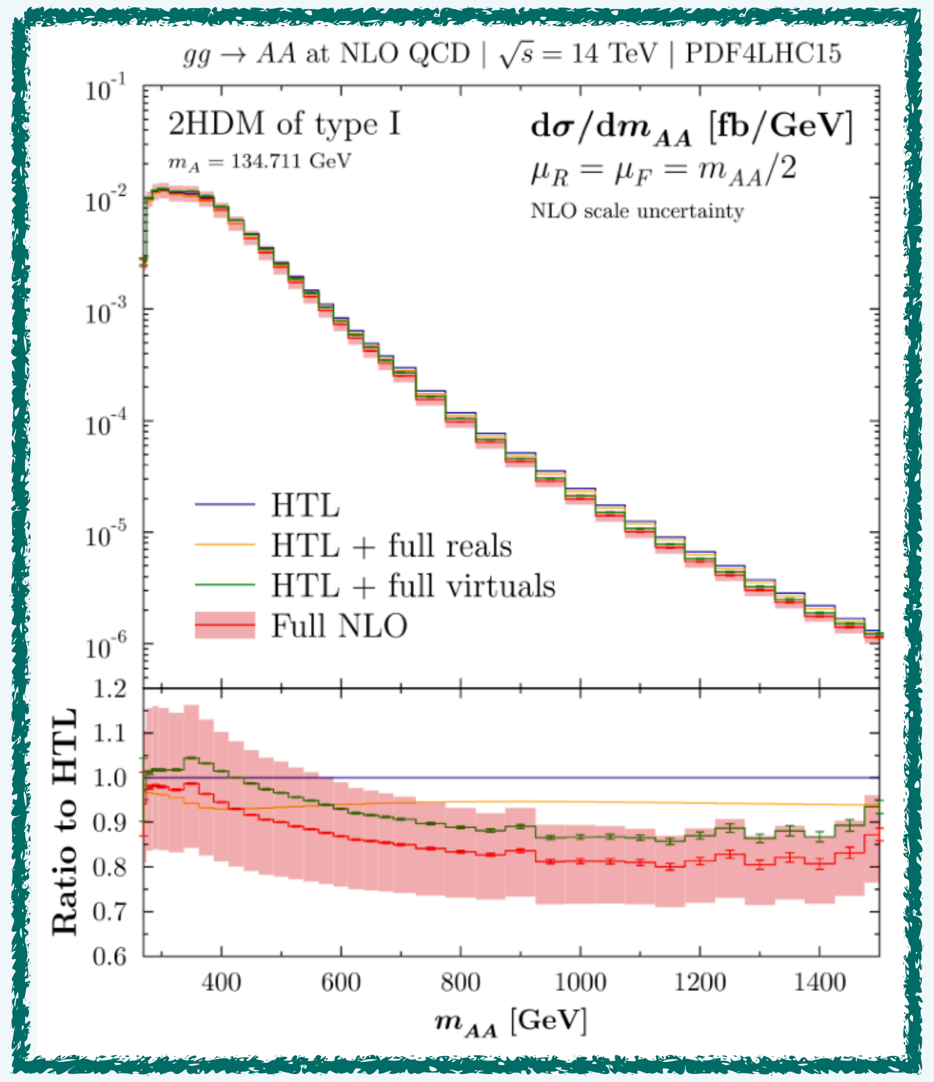
RECEIVED: *March 12, 2020*
REVISED: *April 3, 2020*
ACCEPTED: *April 8, 2020*
PUBLISHED: *April 28, 2020*

Higgs-pair production via gluon fusion at hadron colliders: NLO QCD corrections

Julien Baglio,[a] Francisco Campanario,[b,c] Seraina Glaus,[c,d] Margarete Mühlleitner,[c] Jonathan Ronca,[b] Michael Spira[e] and Juraj Streicher[f]







In-house codes:
- Mathematica
- Fortran 90
- C++

bwForCluster NEMO:
- 900 Nodes
- Broadwell E5-2630 v4
- 128GByte RAM

Calculation size:
- ~million jobs to be run
- %-level precision achieved
- 1 years of running time