# Computational strategies in modern multi-scale two-loop calculations

**Mainz, MathemAmplitudes — September 25, 2023**

ALMA MATER STUDIORUM
UNIVERSITÀ DI BOLOGNA

Theory and Phenomenology
of Fundamental Interactions
UNIVERSITY AND INFN · BOLOGNA

INFN
Istituto Nazionale di Fisica Nucleare

erc

**Tiziano Peraro - University of Bologna and INFN**

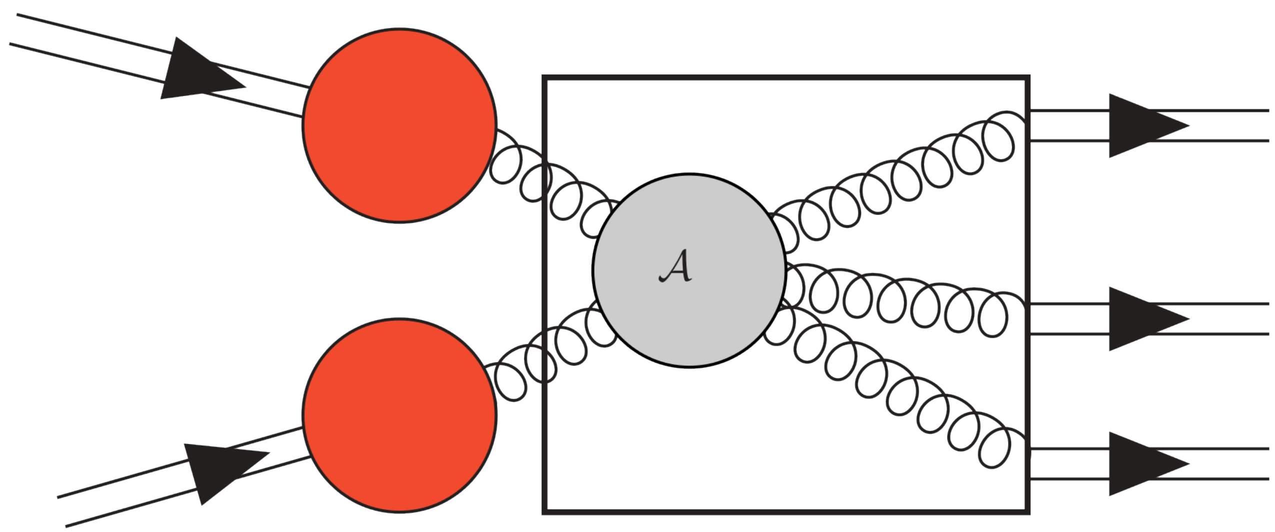
# Motivation

- Theoretical predictions for observables at %-level accuracy
  - search of new physics
  - test SM symmetry breaking mech.

- Crucial understanding of **amplitudes** and **loop integrals**
  - **high-multiplicity** and **massive states** increasingly important
- Exploiting **physical** and **mathematical structures**
  - many connections with fields of mathematics and computing

# Scattering amplitudes

- At the core of **theoretical predictions** in **QFT**




More ingredients:
- PDFs and factorization
- IR subtraction
- resummation
- modelling of other non-pert. effects
- Monte-Carlos and event generators
- etc…

- Can be computed in **perturbation theory**

$$\mathscr{A} = \alpha^k \left(\mathscr{A}_0 + \alpha \mathscr{A}_1 + \alpha^2 \mathscr{A}_2 + \cdots\right)$$

Taylor expansion
in the coupling constants

  - **fixed order**: Feynman diagrams and Feynman rules

# Trees and loops

- **Tree-level** diagrams
  - **rational functions** of kinematic variables (e.g. spinors)
  - contribute (if present) to leading-order (LO) predictions
  - **large uncertainty** and unreliable estimation of it

- **Loop amplitudes** and **loop integrals**
  - **loops** ⇔ **integrals** over unresolved momenta of **virtual particles**
  - contribute at NLO (sometimes LO) and beyond

# Why loops?

- **High-precision** predictions in **high-energy physics**
  - aim at %-level accuracy (compare with LHC data, new physics searches,…)
  - leading-order (LO) predictions have high uncertainty
  - usually next-to-next-to-leading order (NNLO) or better is needed

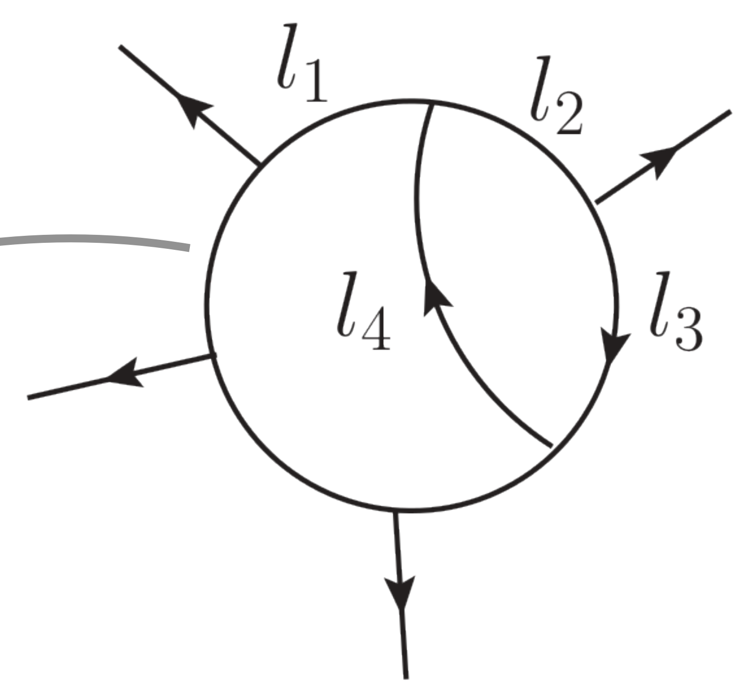
- Loops in QFT and more
  - essential for both **phenomenology** and **theoretical studies** in QFT
  - connections with many fields of **mathematics** (special functions, algebraic geometry, intersection theory), **computing** (number theory, computer algebra, linear algebra, integration) and **physics** (classical observables, gravity)

# Loop calculations

# Loop amplitudes

- At the core of theoretical predictions
- Exhibit rich and interesting mathematical structures
- At the **loop level**, a combination of

$$\mathscr{A} = \int_{-\infty}^{\infty} \left( \prod_{i=1}^{\ell} d^d k_i \right) \frac{\mathscr{N}}{D_1 D_2 D_3 \cdots}$$




Inverse propagators

$$D_j = l_j^2 - m_j^2$$

# Computing loop amplitudes 1/3

- Write **amplitudes** as a linear combination of **loop integrals**

$$\mathcal{A} = \sum_j a_j \; I_j$$

Rational coefficients

Integrals in a “nice/standard” form

- **Standard form** is usually

$$I = \int_{-\infty}^{\infty} \left( \prod_{i=1}^{\ell} d^d k_i \right) \frac{1}{D_1^{\alpha_1} D_2^{\alpha_2} \cdots D_n^{\alpha_n}}, \qquad \alpha_j \lesseqgtr 0$$

INTEGRAL FAMILY
common set of denominators

$D_j =$ inverse propagators + auxiliaries

- **Modern methods**: tensor decomposition, integrand reduction

# Computing loop amplitudes 2/3

Chetyrkin, Tkachov (1981), Laporta (2000)

- Loop integrals obey linear relations, e.g. **IBPs**

$$\int \left(\prod_j d^d k_j\right) \frac{\partial}{\partial k_j^\mu} v^\mu \frac{1}{D_1^{\alpha_1} D_2^{\alpha_2} \cdots} = 0, \qquad v^\mu \in \{p_i^\mu, k_i^\mu\}$$

- Very **large** and sparse linear system => often a **huge bottleneck**
- Solution = **reduction** into a **basis** of linearly independent **master integrals (MIs)** $\{G_j\} \subset \{I_j\}$

$$I_j = \sum c_{jk} G_k$$

rational coefficients

master integrals

# Computing loop amplitudes 3/3

- Computing the **master integrals** (**MIs**)

- Most efficient method is **differential equations**
  **Kotikov (1991), Gehrmann, Remiddi (2000)**

- MIs obey systems of differential equations w.r.t. invariants $x$

$$\partial_x G_j = \sum_k A_{jk} \, G_k$$

  - take **derivates** of MIs and **reduce them to MIs**

  - both analytic and numerical methods

# Analytic vs Algebraic complexity

- **Analytic complexity**
    - understanding space of special functions for amplitudes
    - appears in computation of MIs

- **Algebraic complexity**
    - huge intermediate expressions
    - appears in most steps if we have “many” loops, legs or scales

There’s an interplay between the two!

# Two recent cutting-edge examples

- **Planar loop integrals for massless six-particle scattering**
  **[J. Henn, A. Matijašić, J. Miczajka, T. P., Y. Xu, Y. Zhang (2022-25)**
  **S. Abreu, P. F. Monni, B. Page, J. Usovitsch (2024)]**

  - huge algebraic complexity (6 legs, 8 independent invariants)
  - functional form: iterated integrals of dlog-forms
    (“in principle” well known)

- **Planar loop integrals for top-pair production plus a W boson**
  **[M. Becchetti, D. Canko, V. Chestnov, T. P., M. Pozzoli, S. Zoia (2025)]**

  - algebraic complexity (5 legs, 7 invariants, internal masses)
  - analytic complexity (“elliptic” integrals)

# Finite fields and rational reconstruction

# Finite fields and rational reconstruction

- A successful idea for dealing with **algebraic complexity** **[Kant (2014), von Manteuffel, Schabinger (2014), T.P. (2016)]**
- Reconstruct **analytic results** from **numerical evaluations**
  - intermediate steps are numbers instead of complicated expressions
- Evaluations over **finite fields** $\mathcal{Z}_p$ (computing modulo a **prime** $p$)

$$\mathcal{Z}_p = \{0, 1, \ldots, p - 1\}$$

- Use machine-size integers $p < 2^{64}$ (**fast** and **exact**)
- Collect numerical evaluations and infer **analytic result** form them

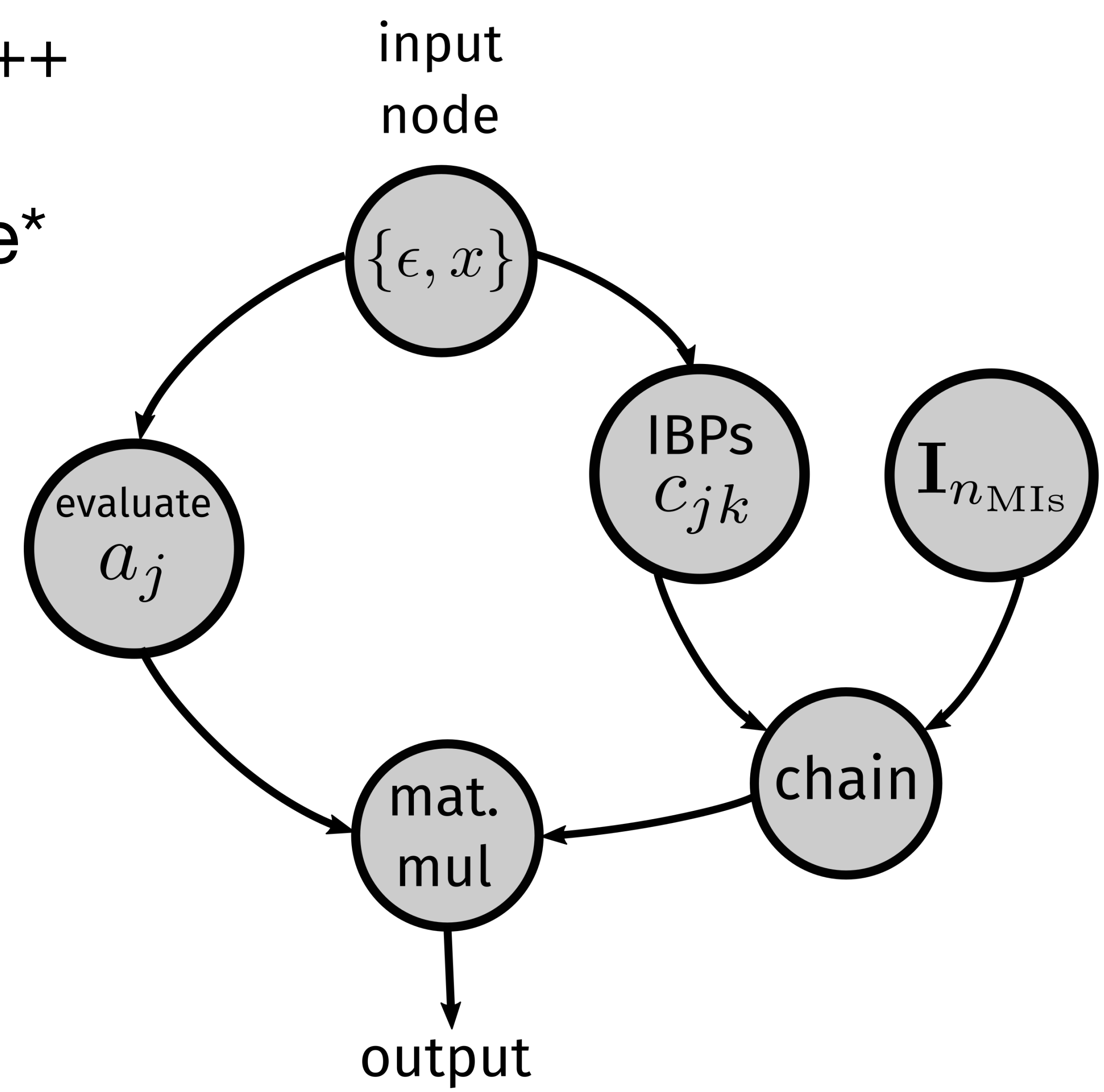
# Finite fields and rational reconstruction

- Applicable to any **rational algorithm**
  - direct reconstruction of **DEs** or **rational coefficients of amplitudes**
- Sidesteps appearance of large intermediate expressions
- Massively **parallelizable**
  - numerical evaluations are independent of each other
  - algorithm-independent parallelization strategy
- Yielded some of the most impressive multi-loop results to date
  - Examples of known codes using it:
    *FinRed, FiniteFlow, FireFly+Kira, Fire, Caravel*
- Useful for both numerical and analytic calculations

# FiniteFlow

T.P. (2019)

- Builds numerical algorithms via a high-level interface
- Combines core algorithms into a computational graph
  - graph evaluation implemented in C++
- Usable as a *Mathematica* package*
  - build efficient implementations of custom algorithms
  - reconstruct analytic results
- Produced many cutting-edge multi-loop results




* Also via a C API or as a Python module (WIP)

# FiniteFlow in the wild

- A flexible framework to implement new algorithms
- Examples of programs using it
  - *FFUtils*, *Symbols*, *LiteIBP* [T.P.] (the latter uses *FiniteFlow+LiteRed* [R.Lee])
  - *AMFlow* [Xiao Liu, Yan-Qing Ma]: numerical evaluation of integrals
  - *Blade* [Guan,Liu,Ma,Wu]: efficient systems for IBP reduction
  - *Initial* [Dlapa,Henn,Yan,Wagner]: finding canonical bases of master integrals
  - *SOFIA* [Correia, Giroux, Mizera] via *Effortless* [A. Matijašić, J. Miczajka]: singularities of loop integrals
  - *CALICO* [Bertolini, Fontana, T.P.]: parametric annihilators and syzygies
  - several private codes for loop integrals, amplitudes and gravity calculations
- Upcoming new version
  - new features, performance and usability improvements (now in `exp` branch)
  - new IBP reduction code: *FFIntRed* [to appear]

# Applications to DEs for loop integrals

# Differential equations (DEs)

- MIs obey systems of differential equations w.r.t. invariants $x$

$$\partial_x \overrightarrow{G} = \sum_k \hat{A}^{(x)}(\epsilon, x) \cdot \overrightarrow{G}$$

- The most well understood case: $\epsilon$-form **[J.Henn (2013)]** with

$$d\overrightarrow{G} = \epsilon \sum_k d\hat{A}(x) \cdot \overrightarrow{G}, \qquad d\hat{A} = \sum_l \hat{c}_j \, d \log w_j(x)$$

  - $w_j =$ algebraic letters, $\{w_j\} =$ alphabet, $\hat{c}_j =$ matrix of rational numbers
  - requires a good choice of MIs (**canonical basis**)

- Integrate order-by-order in $\epsilon$ in terms of iterated integrals

$$\int d \log w_{j_1} \cdots \int d \log w_{j_n}$$

# Reconstructing canonical DEs

- Best case scenario

$$d\overrightarrow{G} = \epsilon \sum_k d\hat{A}(x) \cdot \overrightarrow{G}, \qquad d\hat{A} = \sum_l \hat{c}_j \, d\log w_j(x)$$

  - for a basis $\overrightarrow{G}$ and alphabet $\{w_j\}$ **known a priori**

- Reconstruction of DEs can be drastically simplified
  - take derivatives of MIs
  - reduce them to MIs numerically (over finite fields)
  - numerically "fit" the matrices $\hat{c}_j$ (just a few numerical evaluations!)

- Feasible even for very complex processes
  (e.g. six-particles scattering at two loops)

# Finding canonical bases

## in a nutshell

- **A priori:** integrals with **constant leading singularity**
  - Leading singularity analysis **[J.Henn (2013)]**, by hand or via *DLogBasis* **[P.Wasser]**
  - $d\log$ form in a parametric representation (e.g. Baikov) in $d = 4$

$$I\Big|_{\epsilon=0} = \sum_{j_1,\ldots,j_n} c_{j_1,\ldots,j_n} \int d\log\alpha_{j_1} \cdots \int d\log\alpha_{j_n}, \qquad c_{\vec{j}} \in \mathbb{Q}$$

- **A posteriori:** via a change of basis
  - requires prior analytic reconstruction of DEs (more expensive)
  - Magnus expansion **[Mastrolia, Argeri et al.]**, Fuchsian form etc. **[Henn, Lee, Meyer, Meyer et al.]**

# Finding the alphabet
## in a nutshell

- **Rational** (“even”) letters
  - **singularity analysis** (*BaikovLetters, PLD.jl, SOFIA,* etc…)
  - **denominators** of DEs (requires prior reconstruction)
- **Irrational** (“charged”) letters
  - square roots appear in singularity analysis
  - letters of the form* $w = \dfrac{p + q\sqrt{r}}{p - q\sqrt{r}}$ (see e.g. *Effortless*)
- Understanding **singularity structure** of loop integrals is important

* Products of roots also generally appear

# Canonical DEs, more pragmatically

- **Mix** of different strategies
- Simpler sectors
  - reuse knowledge from simpler processes + changes of bases easier
- More complex sectors
  - analyze on **maximal cuts** first & then correct by lower sectors
  - **check** $\epsilon$-form of DEs by reconstructing only $\epsilon$ dependence
- Realistically and pragmatically
  - analytic reconstruction of **some** matrix elements
  - use information to deduce the other ones up to constants
    + numerical fit via a few numerical evaluations

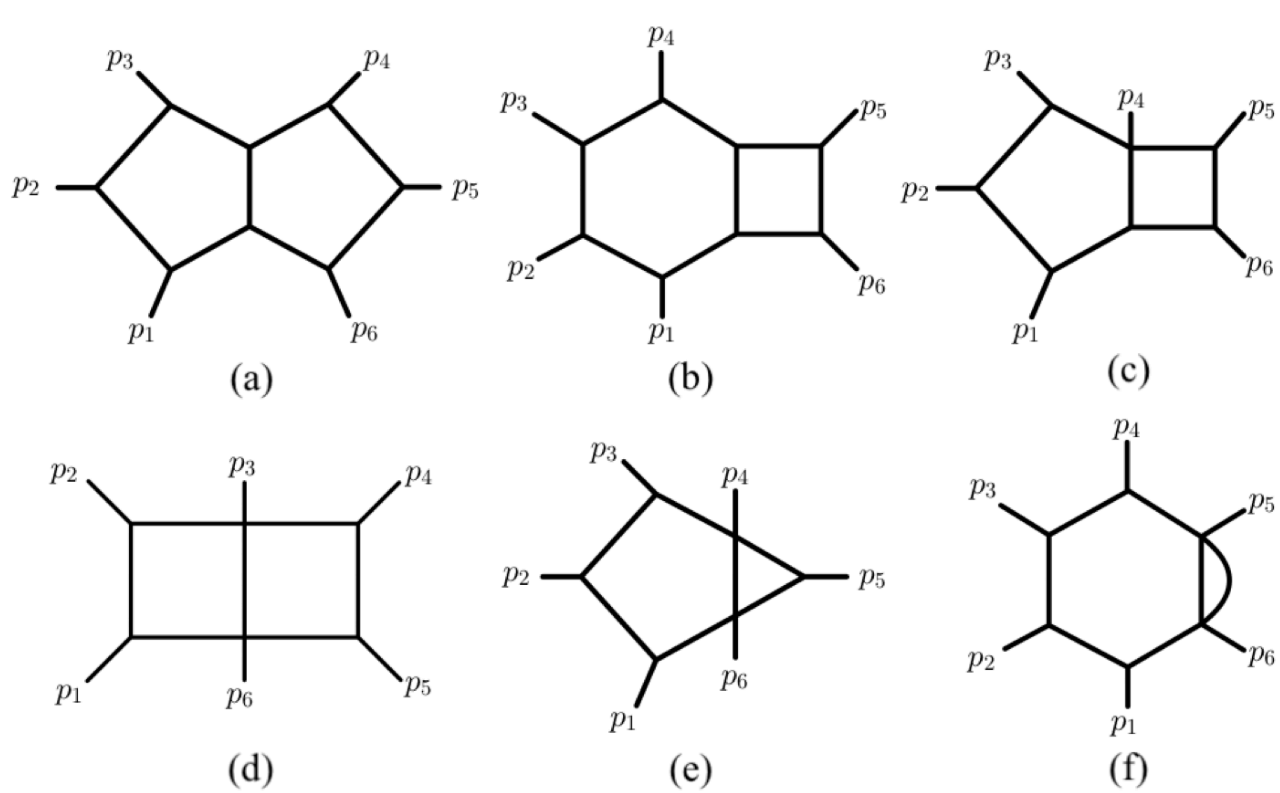
# From DEs to integral evaluation

- Integration in terms of **independent functions**
  - cast in terms of iterated integrals
  - they can be built **systematically** from DEs
    **[Gehrmann, Henn, Lo Presti (2018), Chicherin, Sotnikov (2018), Chicherin, Sotnikov, Zoia (2022), etc…]**
  - can be cast as one-fold integration of logs and $\mathrm{Li}_2$, up to weight 4
  - special functions also satisfy DEs
  - “full” analytic control and efficient numerical evaluation
- **Amplitudes** in terms of independent objects
  - simplifies analytic reconstruction (no “hidden” zeroes)
  - analytic reconstruction still required

# A recent cutting-edge application

**J. Henn, A. Matijašić, J. Miczajka, T. P., Y. Xu, Y. Zhang (2022-25),**
see also **S. Abreu, P. F. Monni, B. Page, J. Usovitsch (2024)**

- Planar two-loop six-particle integrals
  - very high algebraic complexity (8 invariants, 6 legs)
- DEs and numerical evaluation
  - study of its analytic structure made the calculation feasible

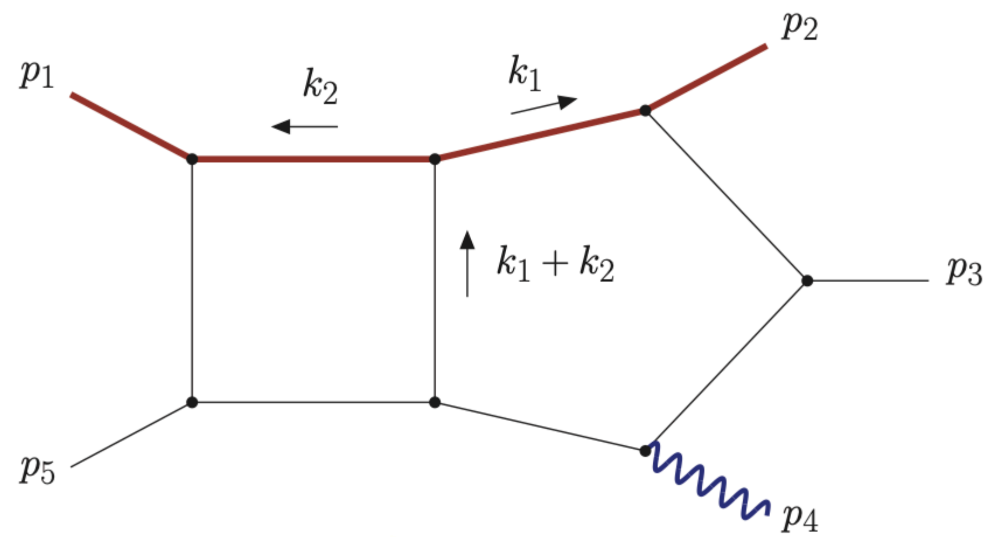


# Increasing the complexity: $t\bar{t} + W$ two-loop integrals

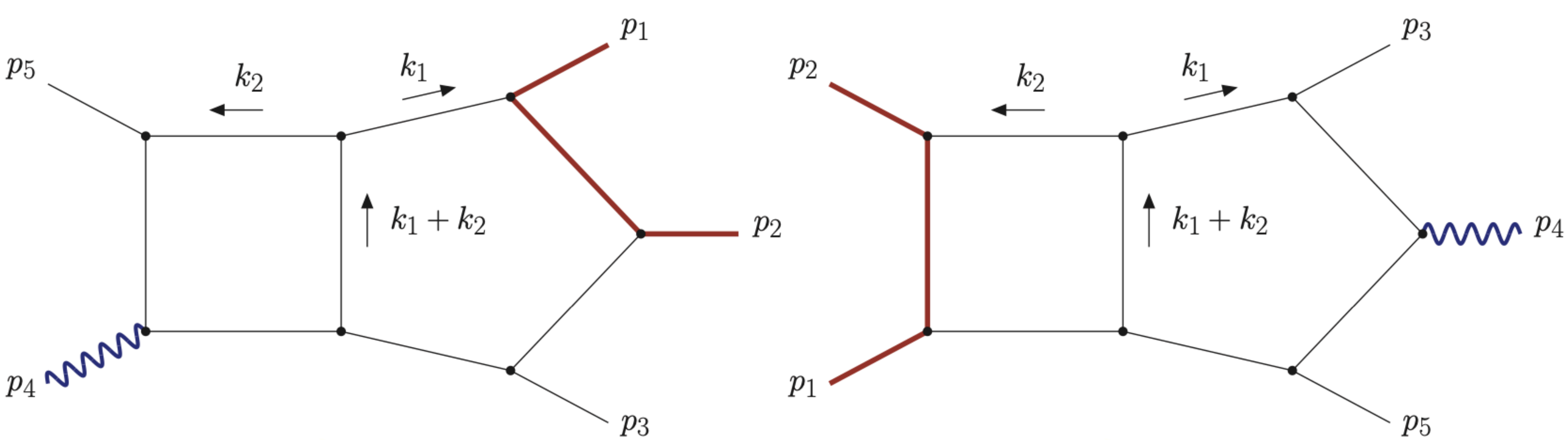
M. Becchetti, D. Canko, V. Chestnov, T. P., M. Pozzoli, S. Zoia (2025)

# Two-loop planar integrals for $t\bar{t} + W$

- Families contributing to $t\bar{t} + W$ production at leading colour




(a) Family $F_1$




(b) Family $F_2$ (c) Family $F_3$

# General strategy for $t\bar{t} + W$

- **Challenge:** huge algebraic complexity paired with higher analytic complexity
- Use "canonical" MIs ($\epsilon$-form) when possible
  - except when it would introduce nested square roots (see later)
- Some sectors are related to **elliptic** geometries
  - $\epsilon$-form would introduce elliptic periods in DEs
  - only done, so far, in algebraically much simpler cases
  - public tools for **numerical evaluations** not supported

➡ aim for DEs with a simple **polynomial form** in $\epsilon$

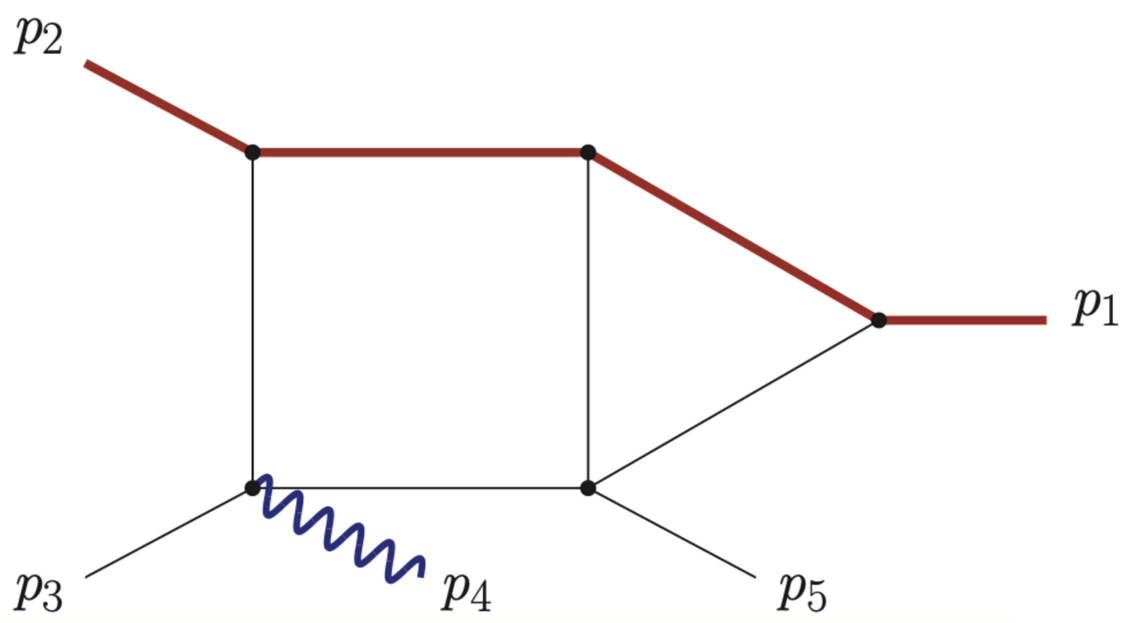
# Nested square roots

- A minor issue arising from leading singularity analysis
- Constant leading singularity would require a normalization with nested roots

$$I \sim \frac{\sqrt{\# + \sqrt{\#}}}{\#} \int d^D k_1 d^D k_2 \cdots$$

- Already observed e.g. in some integrals for $t\bar{t} + H$
  **[Cordero, Figueiredo, Kraus, Page, Reina (2024)]**
- Not an issue, in principle, but public tools for numerical integration don't support them
  - **pragmatic solution**:
    rotate them away at the price of having DEs linear in $\epsilon$
- Not a issue in practice: <u>the main complexity is elsewhere</u>!

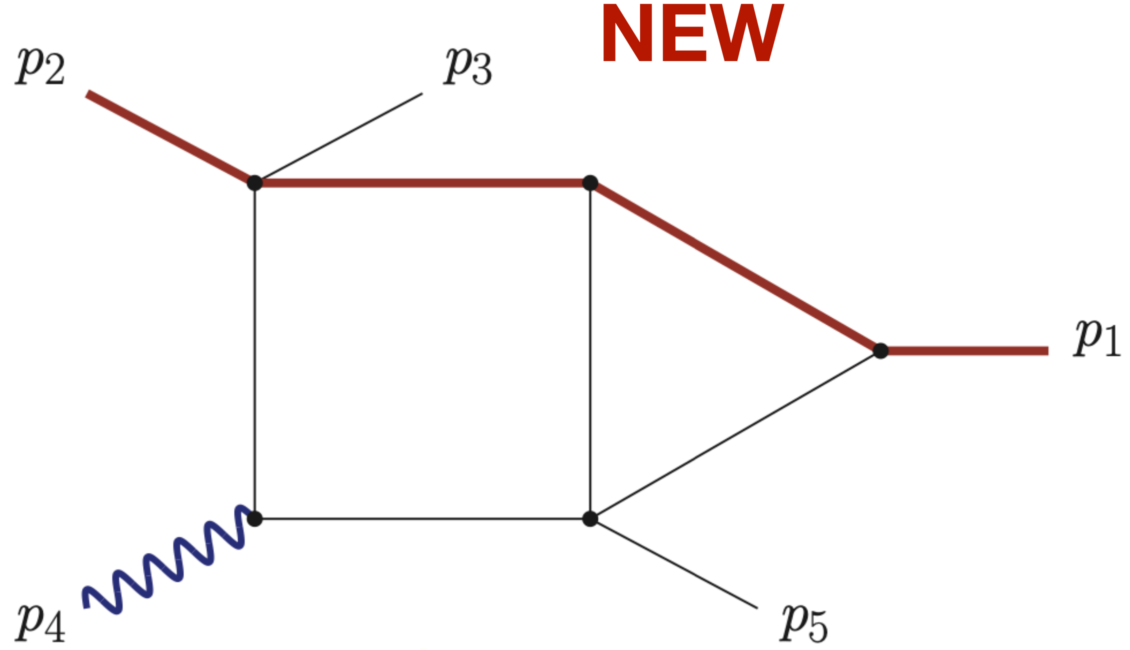
# Elliptic sectors



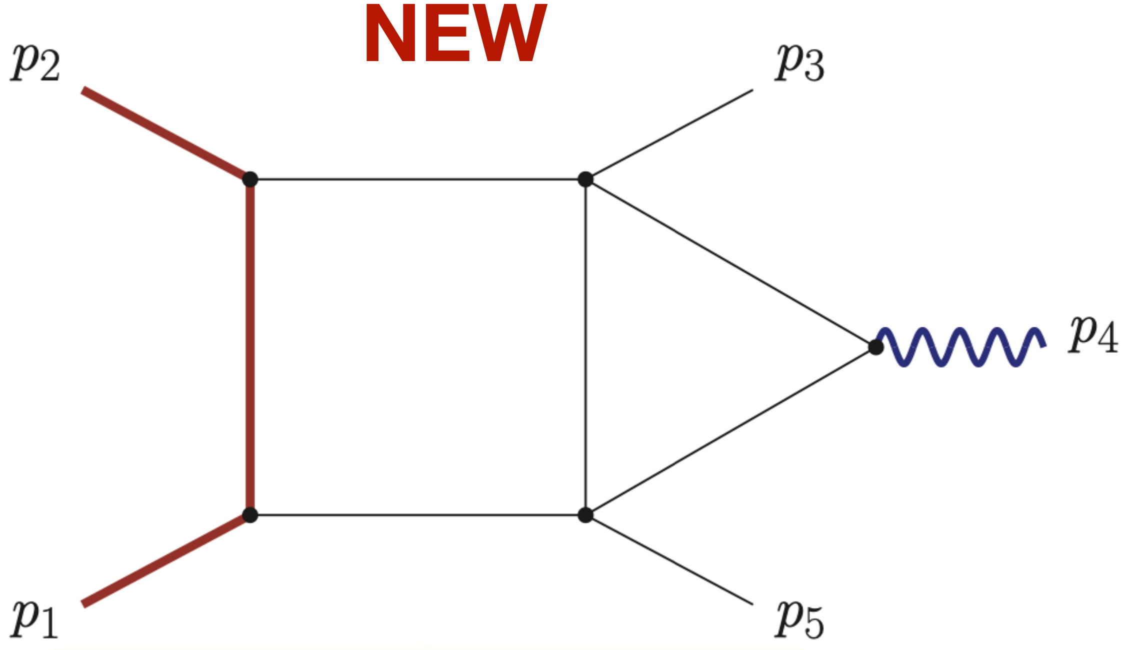

Known from $t\bar{t}+j$

**[Badger,Becchetti, Giraudo,Zoia (2024)]**

**NEW**




**NEW**

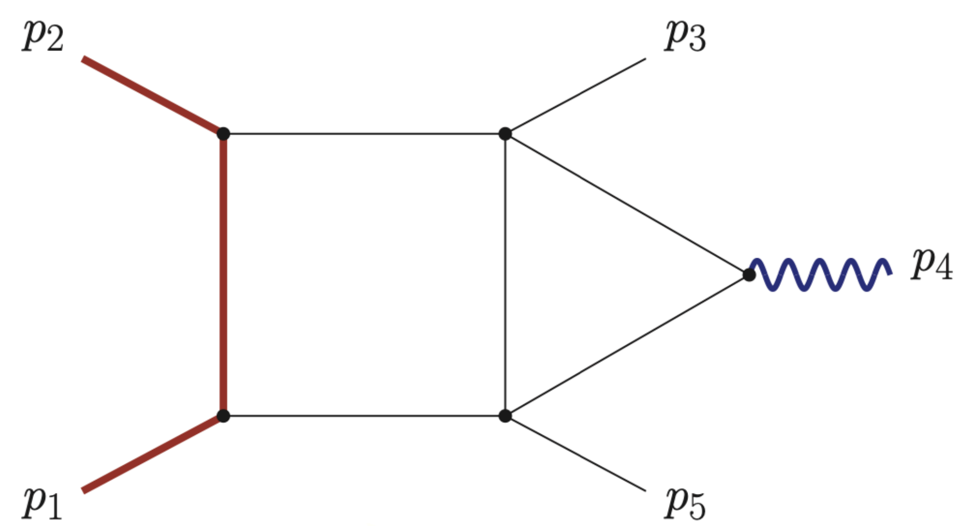


# The most complex sector

see also V.Chestnov's talk

- **Five-point elliptic** sector
- Leading singularity analysis on maximal cut for corner integral yields

$$I \sim \int \frac{dz}{\sqrt{P(z)}} \int d \log \alpha(z, z')$$




- $P(z)$ has degree 4 and describes an **elliptic curve** $y^2 = P(z)$
- the discriminant of $P(z)$ has degree 14 and ~2500 terms
  - appears as denominator of DEs (also cross-checked with *SOFIA*)

# Final form of DEs

- Our final result for DEs takes the form $d\overrightarrow{G} = d\hat{A} \cdot \overrightarrow{G}$ with

$$dA = \sum_{k=0}^{2} \epsilon^k \left( \sum_j \hat{c}_{kj}\, \underline{d \log w_j(x)} + \sum_j \hat{d}_{kj}\, \underline{\omega_j(x)} \right)$$

dlog forms

non-dlog forms $\omega_j(x) = \sum_{a=1}^{7} \omega_{ja}(x)\, dx_a$

- Non-dlog forms contain most of the algebraic complexity
  - irreducible polynomials with up to >550k terms
- MIs chosen to be $O(\epsilon^0)$ and elliptic MIs only contribute at $O(\epsilon^4)$
  - they should only contribute to finite part of amplitudes (modulo algebraic relations we currently don't control)

# Reconstruction of DEs

- No reasonably viable shortcut: **full reconstruction** of DEs
  - direct reconstruction of DEs with *FiniteFlow+FFIntRed* from evaluations over **finite fields**
  - fast numerical evaluations are crucial
- Optimization of IBP reduction: *NeatIBP** **[Z. Wu, J. Boehm, R. Ma, H. Xu, Y. Zhang (2023)]**
  - avoid integrals with higher powers of denominators in identities
  - despite high complexity, *FiniteFlow* reconstructs it on a modern computing node requiring no additional "tricks"
  - a good sign in light of computing amplitudes

* A custom version modified by V. Chestnov that internally uses *FiniteFlow*'s linear solver

# Numerical evaluation of MIs

- A selection of boundary points computed with *AMFlow*
    - slower but only needed for a few points
- Numerical integration from boundary points to physical phases-space
    - we avoid crossing the boundary of physical region
    - various solvers available: *DiffExp*, *Line*, *AMFlow* internal solver

- **Outlook**
    - write DEs in terms of special functions
    - applications to scattering amplitudes and phenomenology

# Conclusions & Outlook

- **Loop integrals** ⇔ mathematical and computational fields
  - algebraic geometry, differential equations, number theory, special functions etc.

- Computational issues in **phenomenologically** motivated problems are tackled using **mathematical knowledge**

- Modern **cutting-edge** calculations use, e.g.
  - **finite fields** and **rational reconstruction**
  - analytic/numerical integration of **differential equations**
  - concepts from **algebraic geometry**