Function bases for canonical differential equations

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UNIVERSITÀ DEGLI STUDI DI TORINO

Outline

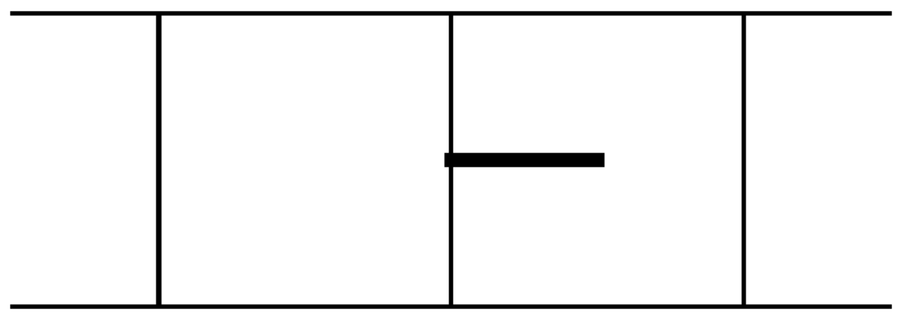
How to solve $$\mathrm{d}\vec{\mathrm{F}}(s;\epsilon) = \epsilon\left[\sum_i A_i\,\mathrm{d}\log W_i(s)\right]\cdot\vec{\mathrm{F}}(s;\epsilon)$$

in an **algorithmic** way such that the solution can be evaluated **efficiently**?

Based on work with

- Chicherin, Sotnikov (2110.10111)
- Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow (2306.15431)

→ Application to 2-loop 5-pt integrals with 1 external mass



Pushing the high-multiplicity frontier of precision LHC physics

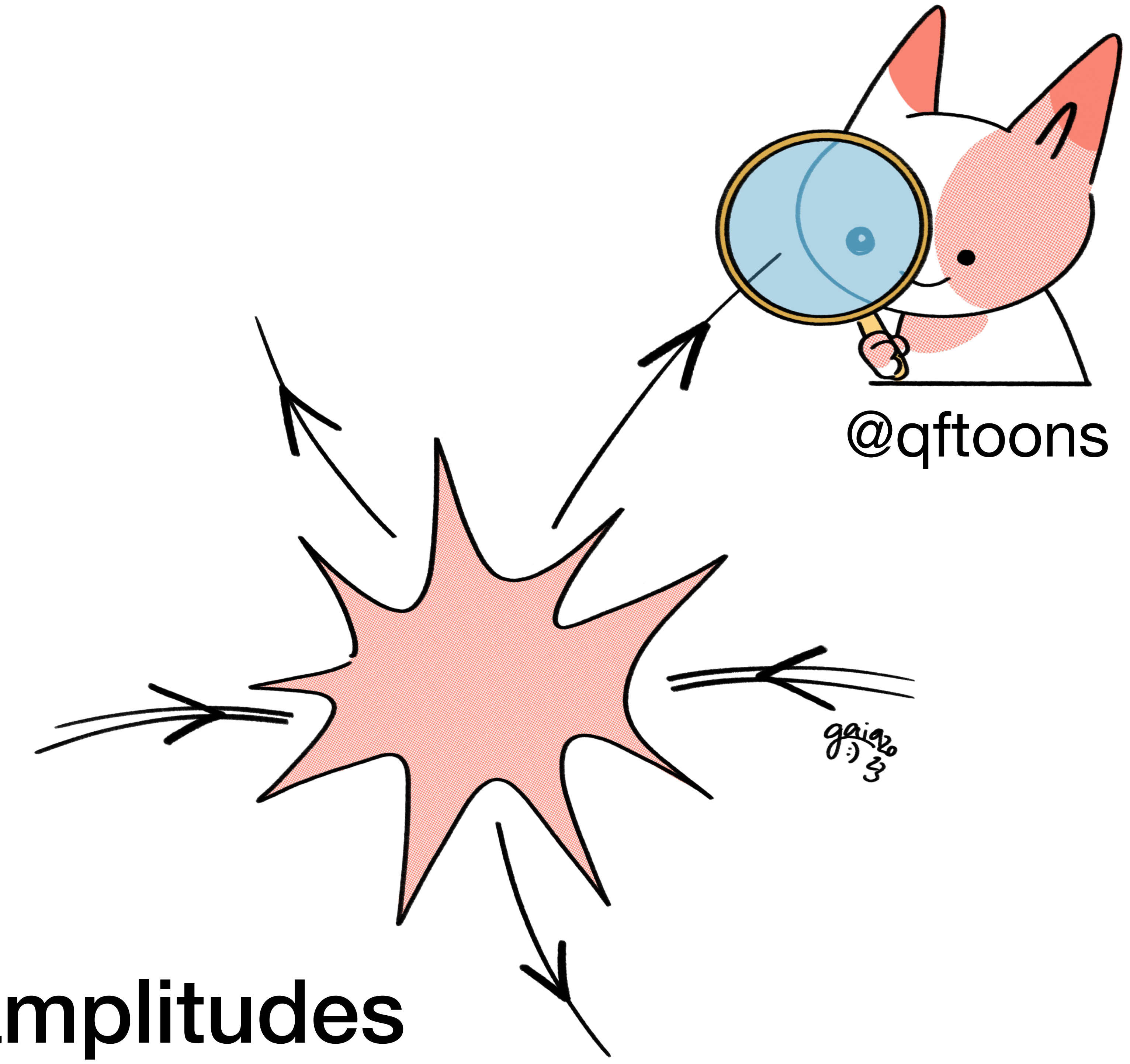
Urgent demand for ~1%-level theoretical predictions: NNLO QCD *at least* is required

Current frontier: 2→3 scattering processes

All massless processes now analysed at NNLO QCD

Next step: adding one mass on the external legs
→ H/W/Z + 2 jet production

Bottleneck: computation of **2-loop 5-pt integrals & amplitudes**



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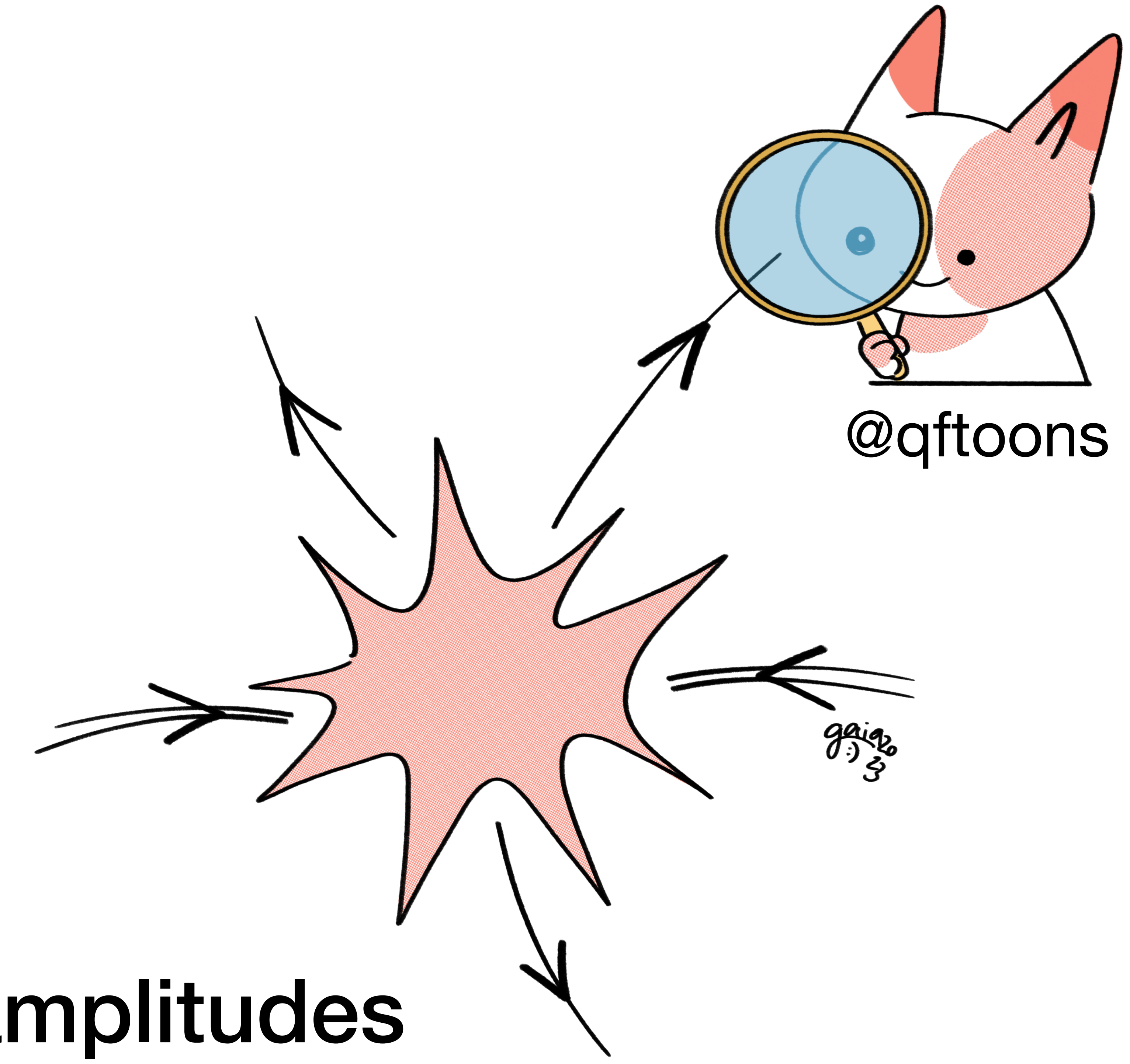
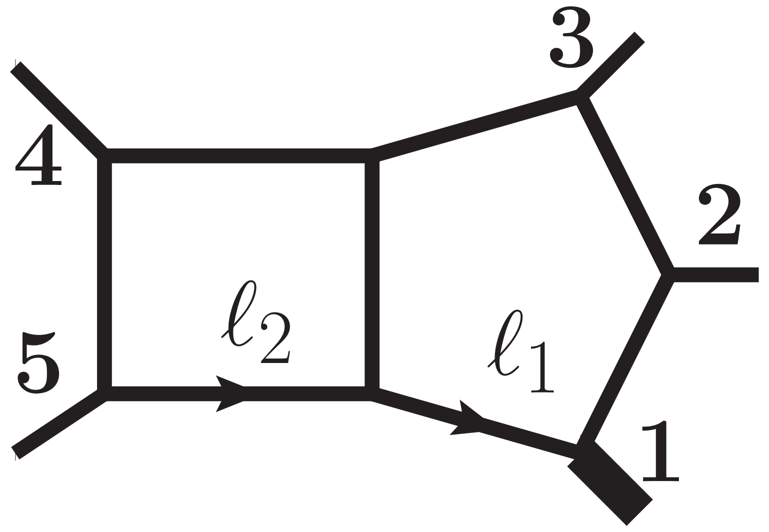


Bottleneck: computation of **2-loop 5-pt integrals & amplitudes**

2-loop 5-pt 1-mass master integrals



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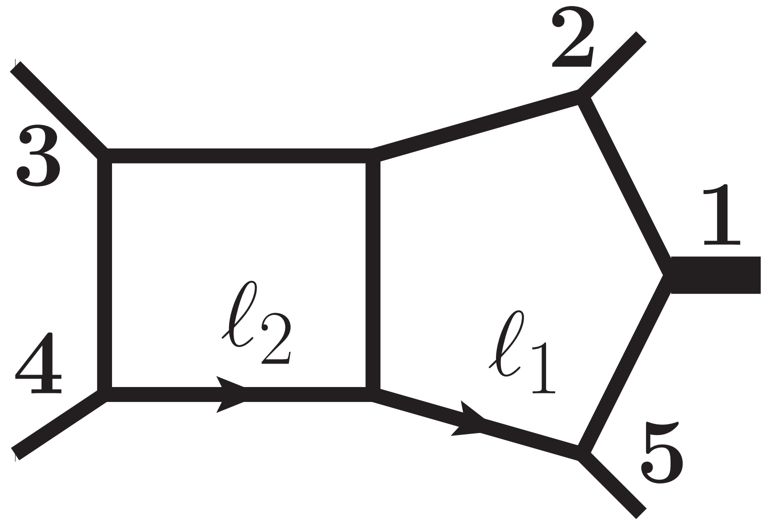

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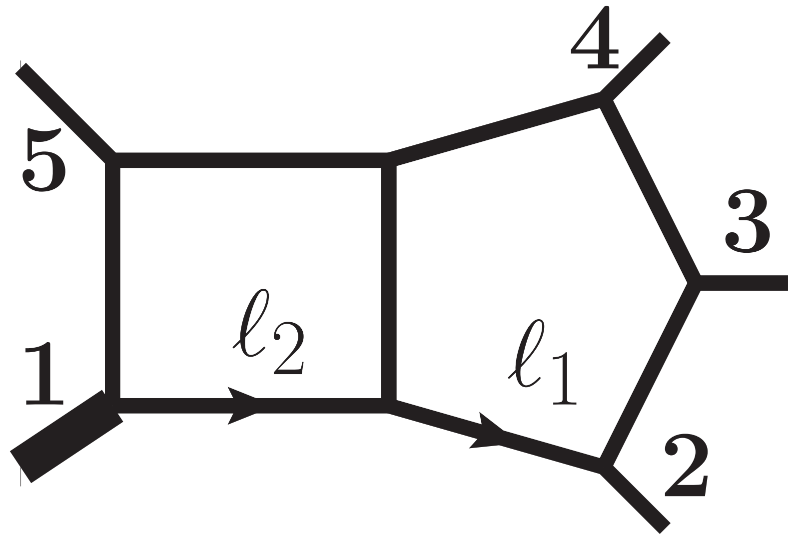

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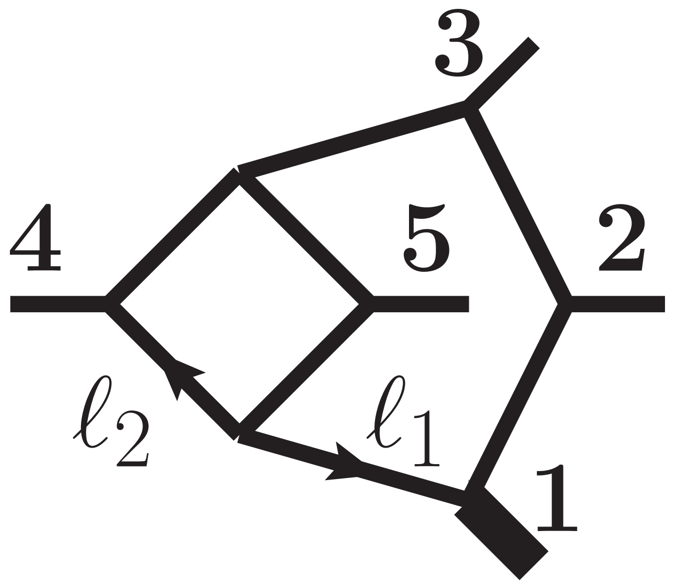
[Abreu, Ita, Moriello, Page, Tschernow, Zeng 2020; Canko, Papadopoulos, Syrrakos 2020; Syrrakos 2020; Chicherin, Sotnikov, **SZ** 2021]



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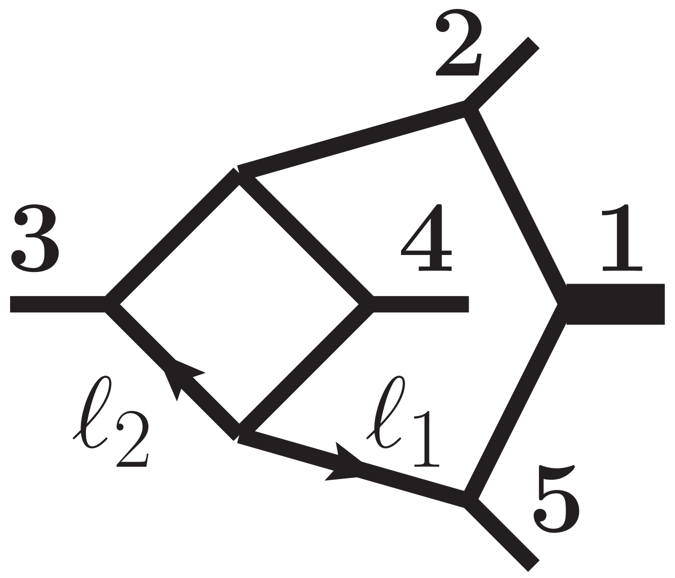

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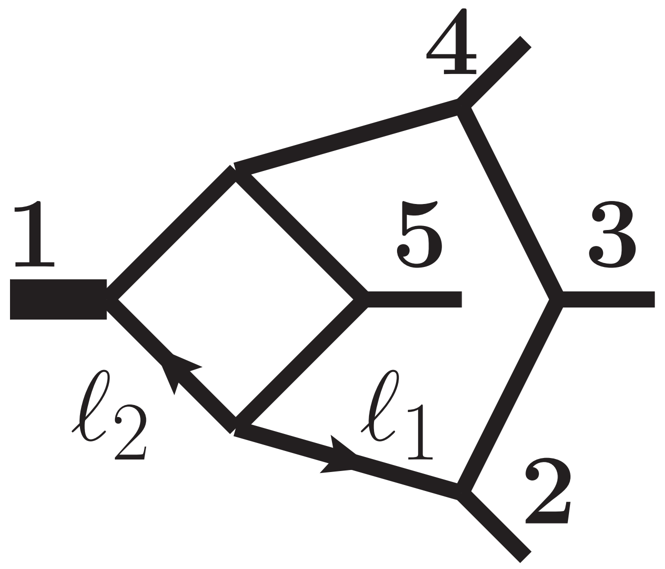

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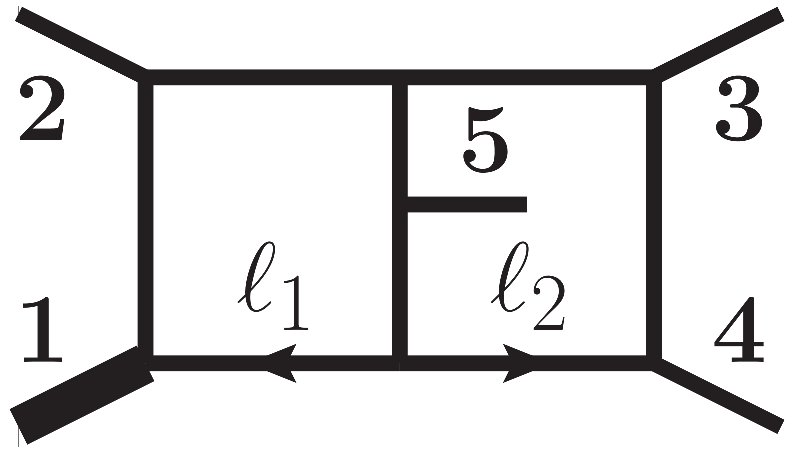
[Abreu, Ita, Moriello, Page, Tschernow 2021; Kardos, Papadopoulos, Smirnov, Syrrakos, Wever 2022]



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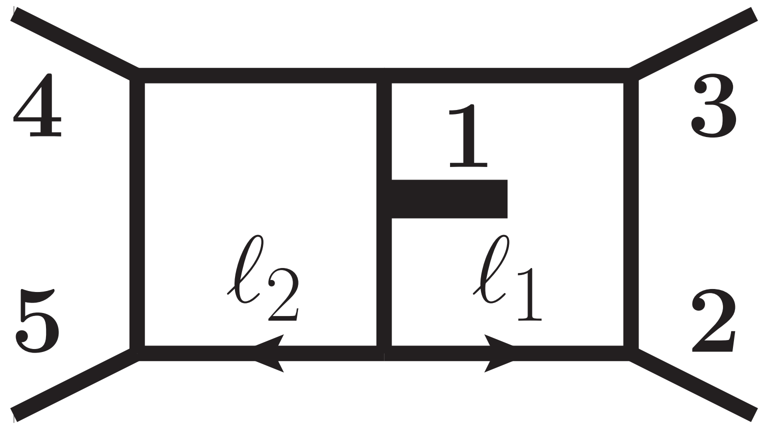

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[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, **SZ** 2023]

Method of differential equations

Integrating by differentiating

[Barucchi, Ponzano ’73; Kotikov ’91; Bern, Dixon, Kosower ‘94; Gehrmann, Remiddi 2000]

$$\frac{\partial}{\partial s_{12}} \overrightarrow{\mathrm{MI}}(s;\epsilon) = A_{s_{12}}(s;\epsilon) \cdot \overrightarrow{\mathrm{MI}}(s;\epsilon)$$

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The **canonical form:**

$$\mathrm{d}\overrightarrow{\mathrm{MI}}(s;\epsilon) = \epsilon \; \mathrm{d}\tilde{A}(s) \cdot \overrightarrow{\mathrm{MI}}(s;\epsilon)$$

[Henn 2013]

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Constant matrices

Letters: algebraic functions of kinematics

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[Henn 2013]

⚠️ Very difficult to obtain, but not part of this talk

$$\tilde{A}(s) = \sum_i a_i \log W_i(s)$$

Constant matrices

Letters: algebraic functions of kinematics

1-mass pentagon alphabet: 204 letters

[Abreu, Ita, Moriello, Page, Tschernow 2021]

127 rational

$$W_1 = p_1^2\,,$$
$$\{W_2,\dots,W_5\} = \{\sigma\,(s_{12}) : \sigma \in S_4/S_3[3,4,5]\}\,,$$
$$\{W_6,\dots,W_{11}\} = \{\sigma\,(s_{23}) : \sigma \in S_4/(S_2[2,3]\times S_2[4,5])\}\,,$$
$$\{W_{12},\dots,W_{15}\} = \{\sigma\,(2\,p_1\cdot p_2) : \sigma \in S_4/S_3[3,4,5]\}\,,$$
$$\{W_{16},\dots,W_{27}\} = \{\sigma\big(2\,p_2\cdot(p_3+p_4)\big) : \sigma \in S_4/S_2[3,4]\}\,,$$

77 algebraic

$$\{W_{186},\dots,W_{188}\} = \left\{\sigma\left(\frac{\Omega^{--}\Omega^{++}}{\Omega^{-+}\Omega^{+-}}\right) : \sigma \in S_4/(S_2[2,3]\times S_2[4,5]\times S_2[s_{23},s_{45}])\right\}\,,$$
$$\{W_{189},\dots,W_{194}\} = \left\{\sigma\left(\frac{\tilde\Omega^{--}\tilde\Omega^{++}}{\tilde\Omega^{-+}\tilde\Omega^{+-}}\right) : \sigma \in S_4/(S_2[3,4]\times S_2[2,5])\right\}\,,$$

where

$$\Omega^{\pm\pm} = s_{12}s_{15} - s_{12}s_{23} - s_{15}s_{45} \pm s_{34}\sqrt{\Delta_3^{(1)}} \pm \sqrt{\Delta_5}\,,$$
$$\tilde\Omega^{\pm\pm} = p_1^2 s_{34} \pm \sqrt{\Delta_5} \pm \sqrt{\Sigma_5^{(1)}}\,,$$

6 variables

10 square roots:

$$\Sigma_5 = (s_{12}s_{15} - s_{12}s_{23} - s_{15}s_{45} + s_{34}s_{45} + s_{23}s_{34})^2 - 4s_{23}s_{34}s_{45}(s_{34} - s_{12} - s_{15})$$

$$\begin{aligned}\Delta_5 &= \det G(p_1,p_2,p_3,p_4)\\ &= (s_{12}s_{15} - s_{12}s_{23} - p_1^2 s_{34} - s_{15}s_{45} + s_{34}s_{45} + s_{23}s_{34})^2\\ &\quad - 4s_{23}s_{34}s_{45}(p_1^2 - s_{12} - s_{15} + s_{34})\,.\end{aligned}$$

Massless case:
31 letters, 1 square root

→ Escalation 😨

Closed under permutations of the massless momenta

How do we solve the DEs?

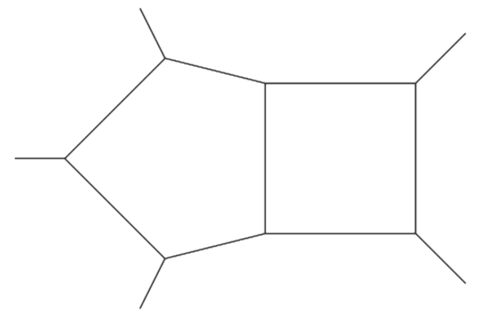
$$\mathrm{d}\vec{\mathrm{F}}(s;\epsilon) = \epsilon\ \mathrm{d}\tilde{A}(s) \cdot \vec{\mathrm{F}}(s;\epsilon)$$

How to solve the DEs?

1. Express MIs in terms of **multiple polylogarithms**

[Canko, Papadopoulos, Syrrakos 2020]

$$G\left(z_1, \ldots, z_n; x\right) = \int_0^x \frac{\mathrm{d}t_1}{t_1 - z_1} \int_0^{t_1} \frac{\mathrm{d}t_2}{t_2 - z_2} \ldots \int_0^{t_{n-1}} \frac{\mathrm{d}t_n}{t_n - z_n}$$



😀 Well understood functions, libraries for numerical evaluation

🙁 Difficult to obtain, functional relations

→ **talks by Torres Bobadilla, Hidding**

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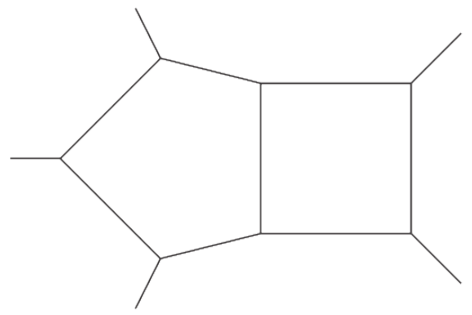

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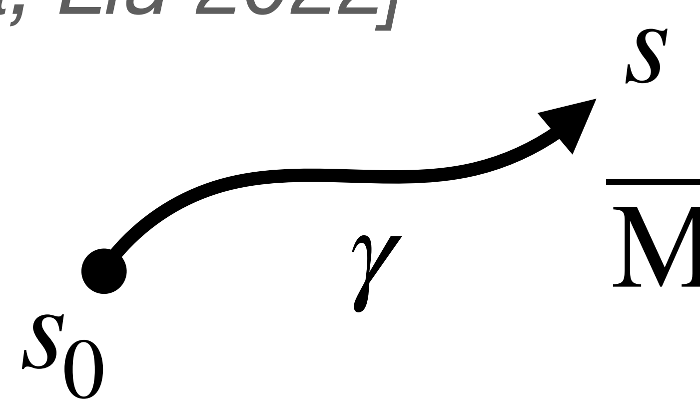
2. Integrate DEs numerically using **generalised series expansions** *[Moriello 2019]*

DiffExp *[Hidding 2020]*, SeaSyde *[Armadillo et al. 2022]*,
AMFlow *[Ma, Liu 2022]*



$\overrightarrow{\mathrm{MI}}\,(s;\epsilon)$

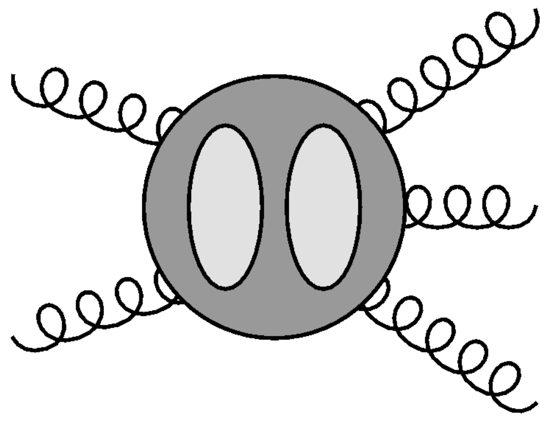
😀 Very flexible and easy to set up

🙁 Time consuming, forced to evaluate the MIs

→ **talks by Ma, Fael**

The “pentagon functions” approach

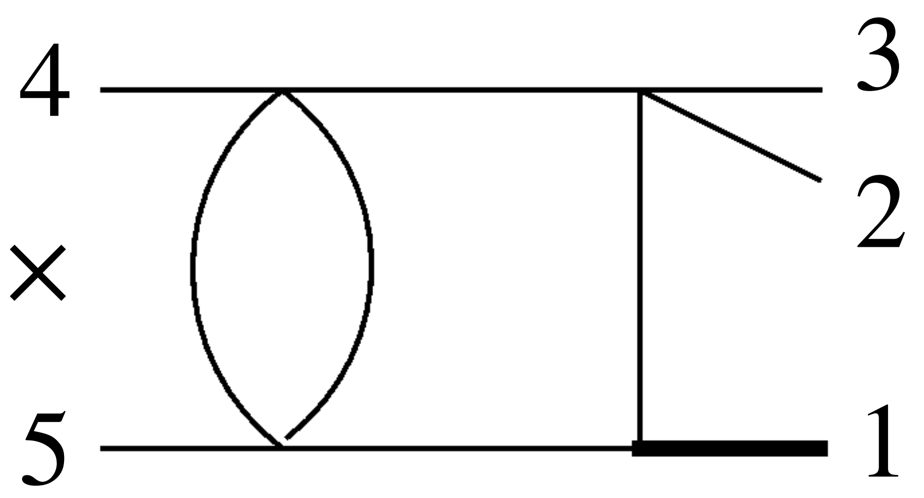
Very successful for massless 2-loop 5-point amplitudes



[Gehrmann, Henn, Lo Presti 2018; Chicherin, Sotnikov 2020]

Construct a **basis** of algebraically independent special functions: $\vec{f} = \{f_i^{(w)}\}$

$$\epsilon^3(1-2\epsilon)\sqrt{\Delta_3^{(1)}}\times$$



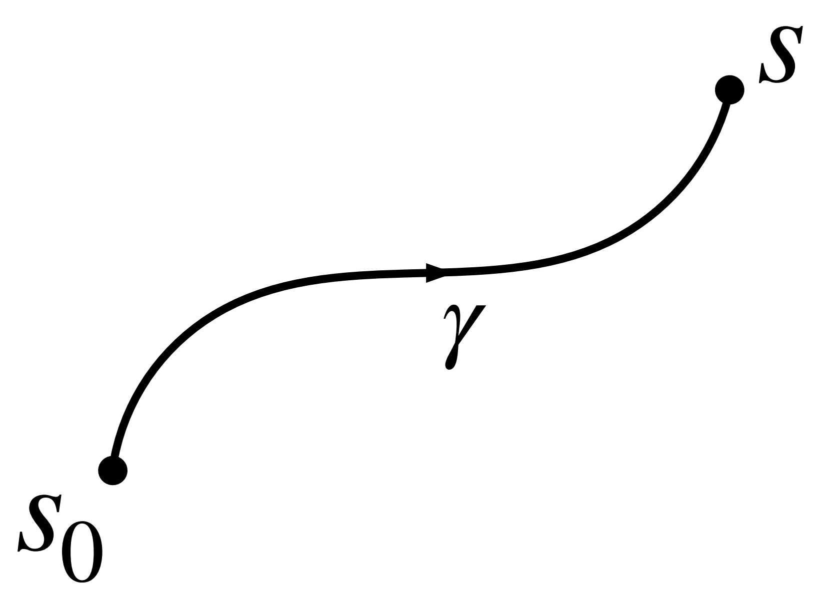
$$= \epsilon^2 f_{23}^{(2)} + \epsilon^3\left[\frac{1}{4}\left(f_1^{(1)} - f_6^{(1)}\right) f_{23}^{(2)} + \frac{1}{2} f_3^{(3)} - \frac{1}{2} f_{29}^{(3)}\right] + \epsilon^4 f_{47}^{(4)} + \mathcal{O}\left(\epsilon^5\right)$$

Efficient numerical evaluation through one-fold integrals

1. Algorithmic construction of the function basis

Chen iterated integrals

→ **talks by Hidding, Pokraka**



$$\left[w_{i_1}, \ldots, w_{i_n}\right]_{s_0}(s) = \int_\gamma \mathrm{d}\log w_{i_n}(s') \left[w_{i_1}, \ldots, w_{i_{n-1}}\right]_{s_0}(s')$$

n = transcendental weight

All functional relations become manifest in terms of iterated integrals

$$\mathrm{Li}_2(z) + \frac{1}{2}\log^2(-z) + \mathrm{Li}_2\left(\frac{1}{z}\right) + \frac{\pi^2}{6} = 0$$

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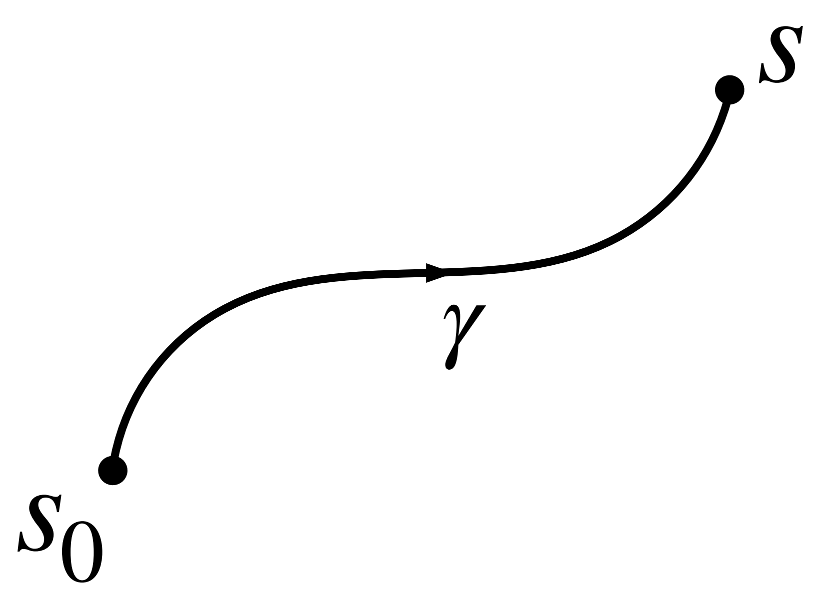

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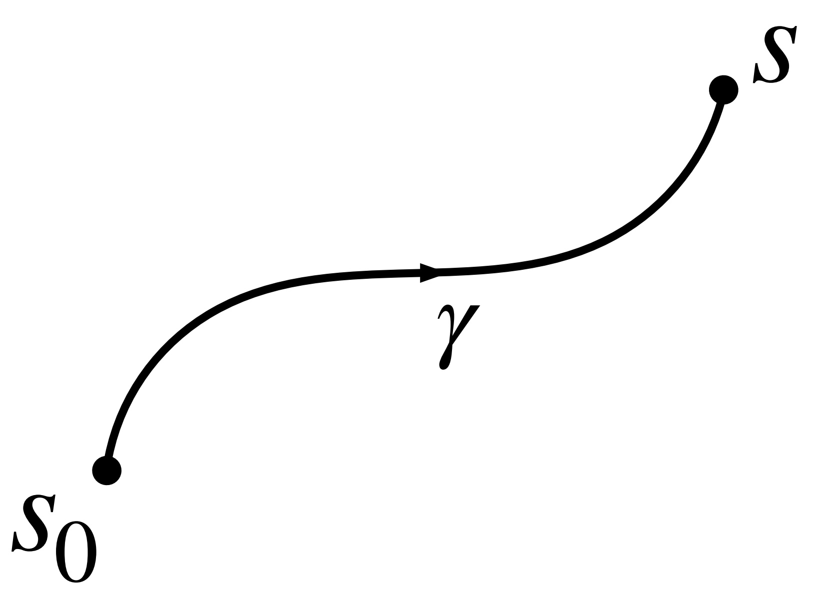

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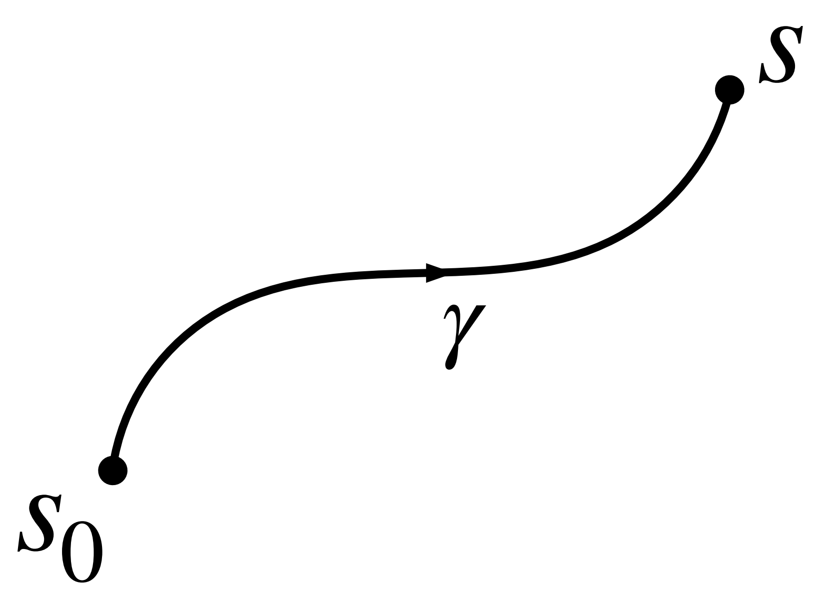

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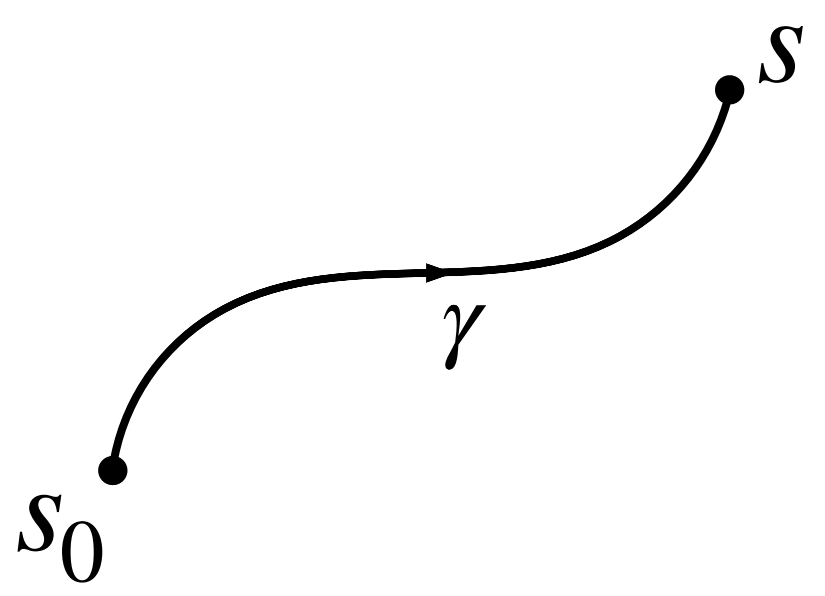

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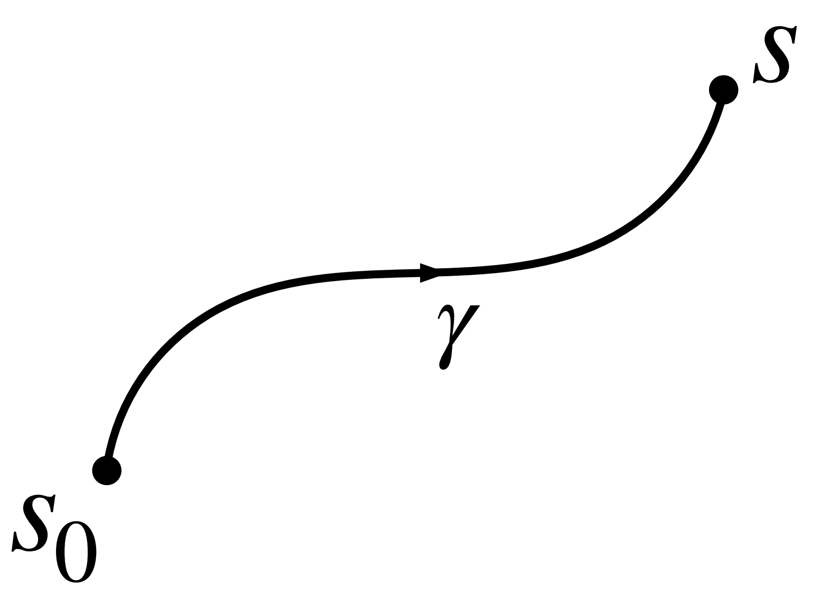

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Solution in terms of Chen iterated integrals can be read off from canonical DEs!

Important properties of iterated integrals

- $\{W_i(s)\}$ multiplicatively independent $\Rightarrow [W_1, \ldots, W_n]$ $\mathbb{Q}$-linearly independent
- No $\mathbb{Q}$-linear relations among iterated integrals with different weight
- Shuffle product:

$$[W_1, W_2]_{s_0} \times [W_3]_{s_0} = [W_1, W_2, W_3]_{s_0} + [W_1, W_3, W_2]_{s_0} + [W_3, W_1, W_2]_{s_0}$$

(weight w_1) $\times$ (weight w_2) $=$ $\mathbb{Q}$-linear combination of weight $(w_1 + w_2)$

Extract function basis from MI coefficients

$$\overrightarrow{\mathrm{MI}}(s,\epsilon) = \sum_{w\geq 0} \epsilon^w \, \overrightarrow{\mathrm{MI}}^{(w)}(s)$$

Written in terms of Chen iterated integrals

Up to required order (here, $w = 4$)

$$\left\{\mathrm{MI}_i^{(1)}\right\} \longrightarrow \left\{f_k^{(1)}\right\}$$

$$\left\{\mathrm{MI}_i^{(2)}\right\} \cup \left\{f_i^{(1)} \times f_j^{(1)}\right\} \longrightarrow \left\{f_k^{(2)}\right\}$$

$$\left\{\mathrm{MI}_i^{(3)}\right\} \cup \left\{f_i^{(2)} \times f_j^{(1)}\right\} \cup \left\{f_i^{(1)} \times f_j^{(1)} \times f_k^{(1)}\right\} \longrightarrow \left\{f_k^{(3)}\right\}$$

$$\left\{f_i^{(w)}\right\}_{i,w=1,\ldots,4}$$

Algebraically independent

Irreducible

Solution of a linear system of equations

Linear algebra only 👍

Need to know relations among boundary values

We only know $\overrightarrow{\mathrm{MI}}^{(w)}(s_0)$ numerically

Previous approach: high-precision evaluation of MPLs + PSLQ algorithm

[Ferguson, Bailey '92]

$$\mathrm{MI}_1^{(2)}(s_0) = -\,1.644934067\ldots$$
$$\mathrm{MI}_2^{(2)}(s_0) = 0.4060916335\ldots$$
$$\mathrm{MI}_3^{(2)}(s_0) = 1.436746367\ldots$$

$$\longrightarrow \quad 3\,\mathrm{MI}_1^{(2)}(s_0) + 4\,\mathrm{MI}_2^{(2)}(s_0) - 2\,\mathrm{MI}_3^{(2)}(s_0) = 0$$

- Very heavy from computational point of view (e.g. ~3000-digit precision in *[Chicherin, Sotnikov, **SZ** 2021]*) 😕
- Relies on MPL representation ☹️

The new algorithm

*[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, **SZ** 2023]*

1. Select MI coefficients for the basis at **symbol** level $\left\{f_i^{(w)}\right\}$ *[Goncharov, Spradlin, Vergu, Volovich 2010]*

Symbol = iterated integral stripped of boundary information → **talk by Dixon**

$$\mathrm{Li}_2(z) = -\left[1-z, z\right]_{-1} - \log 2\left[z\right]_{-1} - \frac{\pi^2}{12} \longrightarrow \mathcal{S}\left[\mathrm{Li}_2(z)\right] = -\left[1-z, z\right]$$

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2. **Ansatz**: all MI coefficients are polynomials in $\left\{f_i^{(w)}\right\}$ + ζ_2 and ζ_3 (up to weight 4)

$$\mathrm{MI}^{(2)} = \sum_i \alpha_i f_i^{(2)} + \sum_{i\leq j} \beta_{ij} f_i^{(1)} f_i^{(1)} + \gamma\,\zeta_2 \qquad \alpha_i, \beta_{ij}, \gamma \in \mathbb{Q}$$

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$$\mathrm{Li}_2(z) = -\left[1-z, z\right]_{-1} - \log 2\left[z\right]_{-1} - \frac{\pi^2}{12} \longrightarrow \mathcal{S}\left[\mathrm{Li}_2(z)\right] = -\left[1-z, z\right]$$

2. **Ansatz**: all MI coefficients are polynomials in $\left\{f_i^{(w)}\right\}$ + ζ_2 and ζ_3 (up to weight 4)

$$\mathrm{MI}^{(2)} = \sum_i \alpha_i f_i^{(2)} + \sum_{i \le j} \beta_{ij} f_i^{(1)} f_i^{(1)} + \gamma\, \zeta_2 \qquad \alpha_i, \beta_{ij}, \gamma \in \mathbb{Q}$$

Fixed by symbol-level analysis

The new algorithm

[Abreu, Chicherin, Ita, Page, Sotnikov, Tschernow, **SZ** 2023]

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Fixed by symbol-level analysis (α_i, β_{ij})

Fixed by evaluation at s_0 + rationalisation (γ)

Summary of the algorithm

Input:
- canonical DEs
- numerical boundary values $\{\mathrm{MI}_i^{(w)}(s_0)\}$

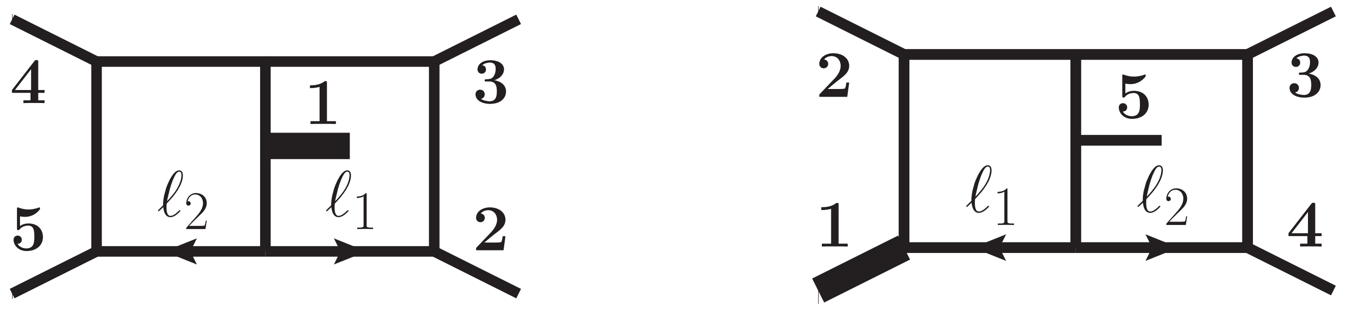
Only needed at the accuracy required for the evaluation (~70 digits)

Easy to obtain using **AMFlow** → **talk by Ma**

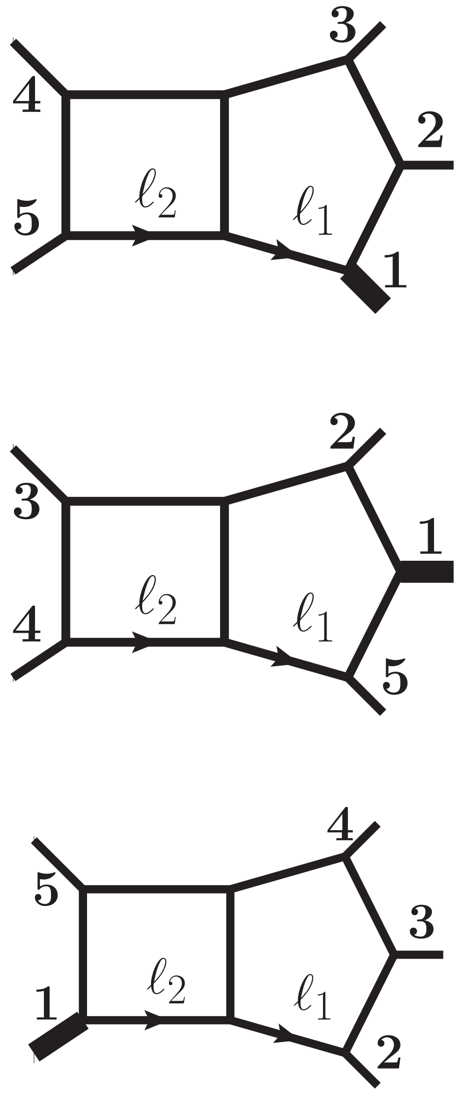
[Liu, Ma 2022]

Output:
- function basis $\{f_i^{(w)}\}$ (written in terms of iterated integrals)
- relations among the boundary values
- expression of all MI coefficients as polynomials in $\{f_i^{(w)}\}$ and ζ values

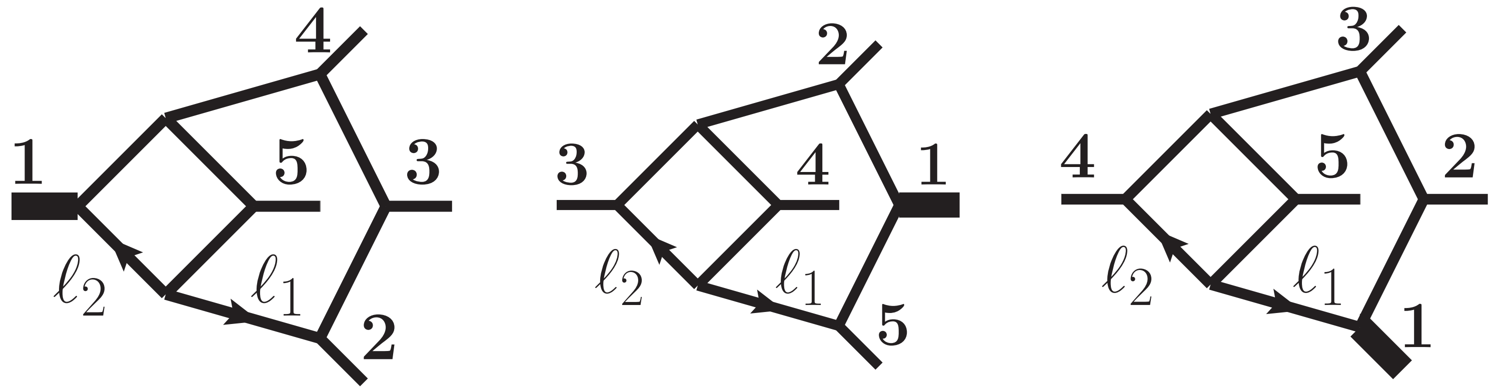
One-mass pentagon functions



All 1-mass 2-loop 5-pt integrals



weight	P ∪ PB	HB	DP	Total
1	11	0	0	11
2	25	10	0	35
3	145	72	0	217
4	675	305	48	1028



Functions chosen to highlight analytic properties

E.g. letters expected to drop out, singularities… are isolated in the minimal number of functions

All 4! permutations of external massless legs → everything that is needed for any amplitude of this kind

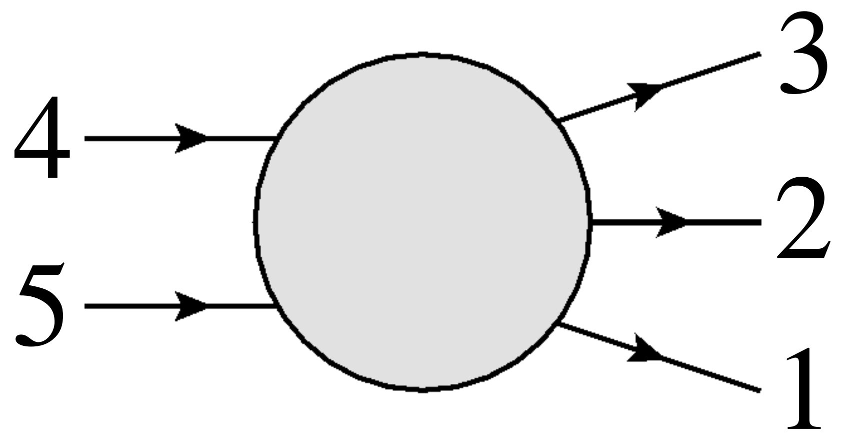
2. Efficient numerical evaluation

Logs and dilogarithms up to weight 2

Explicit expressions by fitting ansätze

$$f^{(1)} \sim \log + \tau^{(1)}$$
$$f^{(2)} \sim \mathrm{Li}_2 + \log^2 + \tau^{(1)} \log + \tau^{(2)}$$

Arguments guessed *[Duhr, Gangl, Rhodes 2011]* and chosen s.t. functions are well defined in a physical scattering region (s_{45} channel)



$$f_2^{(1)} = \log\left(-s_{34}\right)$$
$$f_2^{(2)} = \mathrm{Li}_2\left(\frac{s_{14}}{p_1^2}\right) + \log\left(-\frac{s_{14}}{p_1^2}\right)\log\left(1-\frac{s_{14}}{p_1^2}\right) + \mathrm{i}\pi \log\left(s_{15} - s_{23} + s_{45}\right) - \mathrm{i}\pi \log\left(p_1^2\right)$$

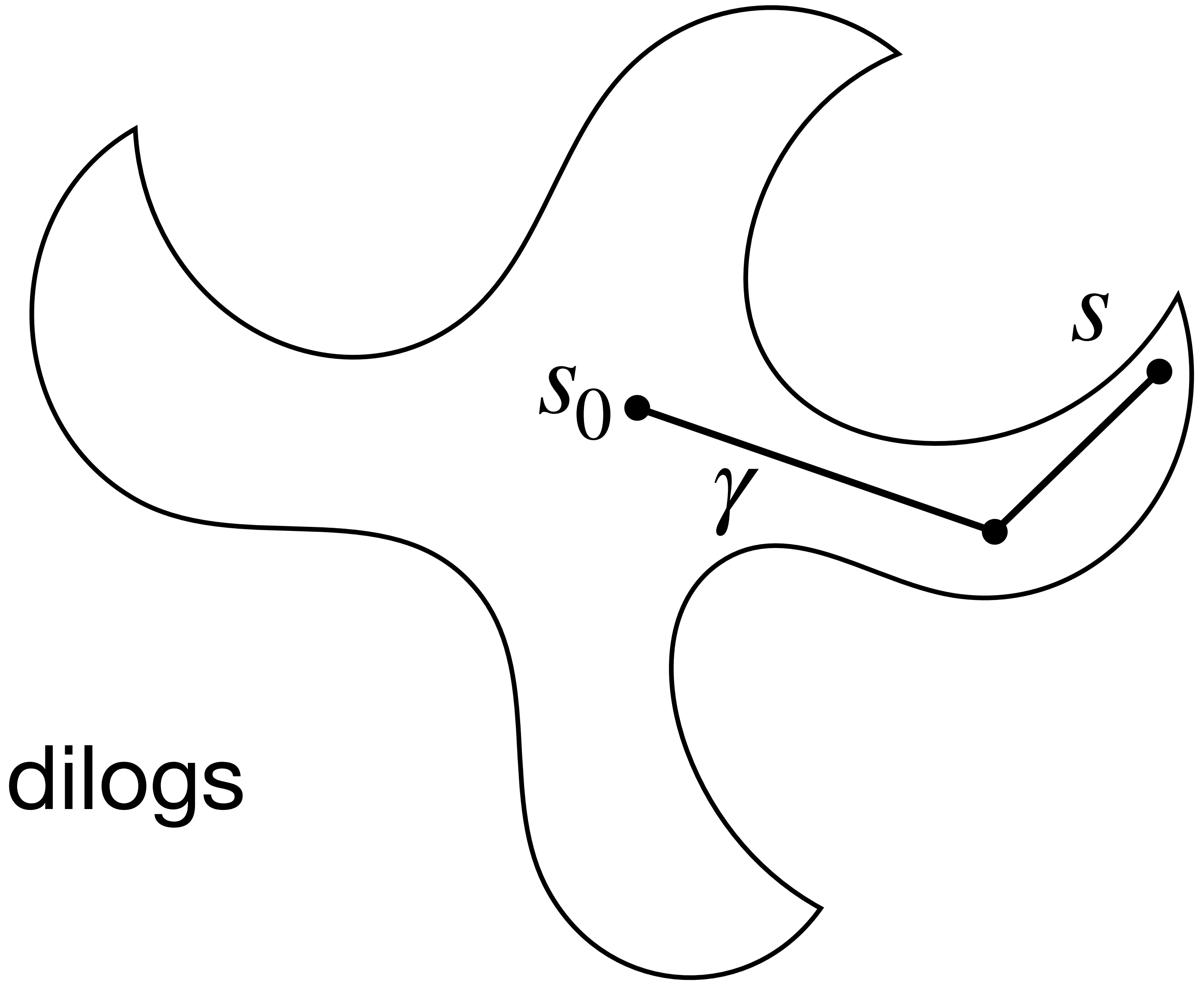
Can be evaluated numerically straightforwardly

One-fold integrals at weight 3 and 4

Path $\gamma : [0,1] \to s$ entirely within the physical region

$$\left[W_{i_1}, W_{i_2}, W_{i_3}\right]_{s_0}(s) = \int_0^1 \mathrm{d}t\, \frac{\mathrm{d}\log W_{i_3}\left(s'(t)\right)}{\mathrm{d}t} \left[W_{i_1}, W_{i_2}\right]_{s_0}\left(s'(t)\right)$$

Logs and dilogs



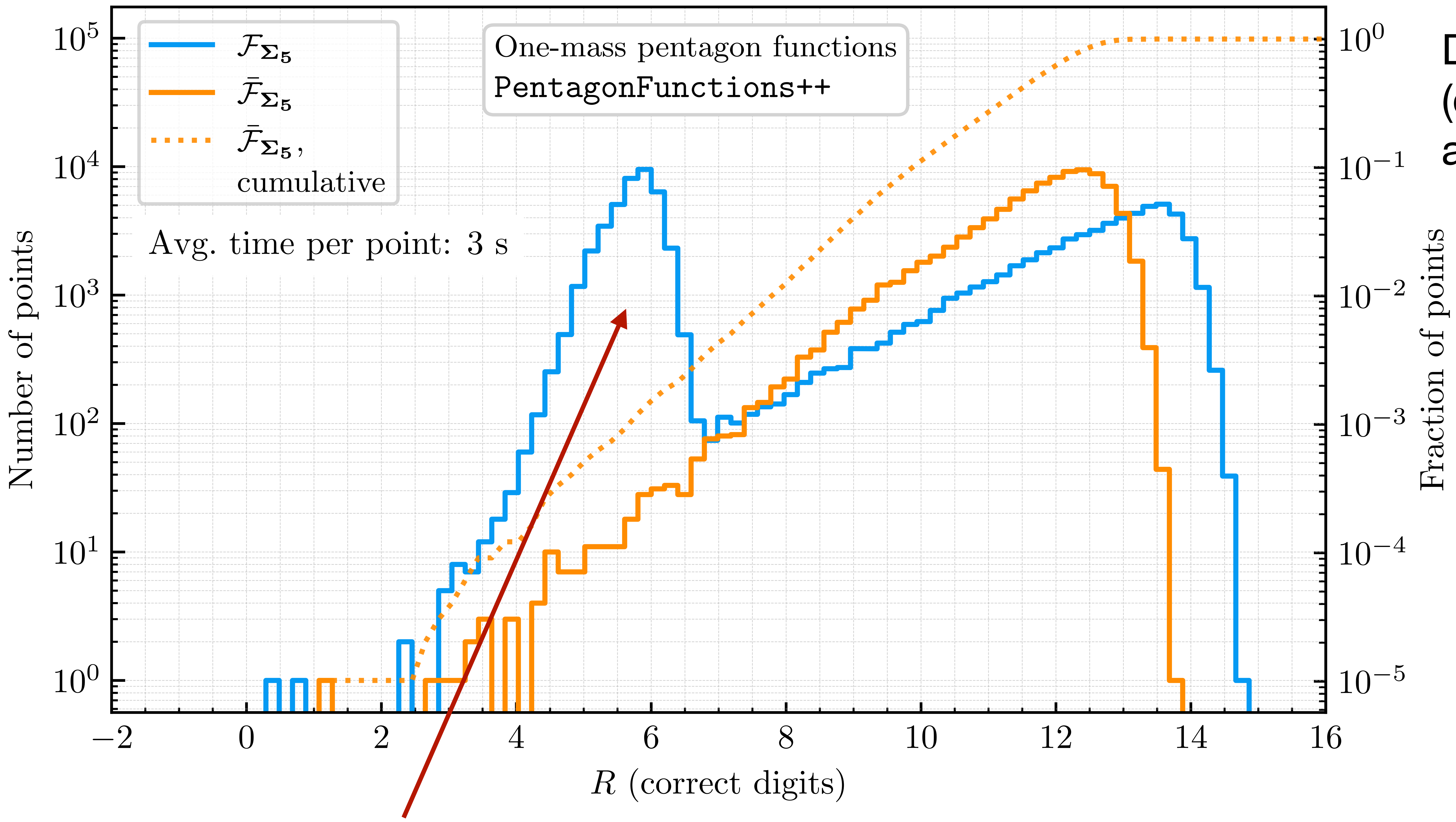
s_{45} channel

Through integration by parts *[Caron-Huot, Henn 2014]*

$$f^{(4)} \sim \int_0^1 \mathrm{d}t\, \log \times \frac{\mathrm{d}\log}{\mathrm{d}t} \times f^{(2)}$$

No analytic continuation required!

Numerical integration implemented in C++ library **PentagonFunctions++**



Double accuracy (quadruple and octuple also available)

New non-planar feature: integrable (and genuine) singularities in the s_{45} channel at $\Sigma_5^{(i)} = 0$

Planar subset ~10 times better

Pentagon functions and finite fields methods allowed for efficient computation of amplitudes

Massless pentagon functions

[Chicherin, Sotnikov 2020]

- 3γ *[Abreu, Page, Pascual, Sotnikov 2020; Chawdhry, Czakon, Mitov, Poncelet 2021; Abreu, De Laurentis, Ita, Klinkert, Page, Sotnikov, 2023]*
- $2\gamma + \mathrm{j}$ *[Agarwal, Buccioni, von Manteuffel, Tancredi 2021; Chawdhry, Czakon, Mitov, Poncelet 2021; Badger, Brönnum-Hansen, Chicherin, Gehrmann, Hartanto, Henn, Marcoli, Moodie, Peraro, **SZ** 2021]*
- $3\mathrm{j}$ (planar) *[Abreu, Febres-Cordero, Ita, Page, Sotnikov 2021]*
- $\gamma + 2\mathrm{j}$ *[Badger, Czakon, Bayu Hartanto, Moodie, Peraro, Poncelet, **SZ** 2023]*

1-mass pentagon functions (planar)

*[Chicherin, Sotnikov, **SZ** 2021]*

- $\mathrm{W} + \mathrm{b}\bar{\mathrm{b}}$ (planar) *[Badger, Bayu Hartanto, **SZ** 2021; Bayu Hartanto, Poncelet, Popescu, **SZ** 2022]*
- $\mathrm{W} + 2\mathrm{j}$ (planar) *[Abreu, Febres Cordero, Ita, Klinkert, Page, Sotnikov 2022]*
- $\mathrm{H} + \mathrm{b}\bar{\mathrm{b}}$ (planar) *[Badger, Bayu Hartanto, Kryś, **SZ** 2021]*
- $\mathrm{W} + \gamma + \mathrm{j}$ (planar) *[Badger, Bayu Hartanto, Kryś, **SZ** 2022]*

→ talks by von Manteuffel, de Laurentis

Ready for deployment in NNLO QCD phenomenology

Leading colour @ 2 loops

$pp \to 3\gamma$ *[Kallweit, Sotnikov, Wiesemann 2020; Chawdhry, Czakon, Mitov, Poncelet 2020]*

$pp \to 2\gamma + j$ *[Chawdhry, Czakon, Mitov, Poncelet 2021; Badger, Gehrmann, Marcoli, Moodie 2021]*

$pp \to 3j$ *[Czakon, Mitov, Poncelet 2021; Chen, Gehrmann, Glover, Huss, Marcoli 2022]*

$pp \to W + b\bar{b}$ *[Bayu Hartanto, Poncelet, Popescu, **SZ** 2022; Buonocore, Devoto, Kallweit, Mazzitelli, Rottoli, Savoini 2023]*

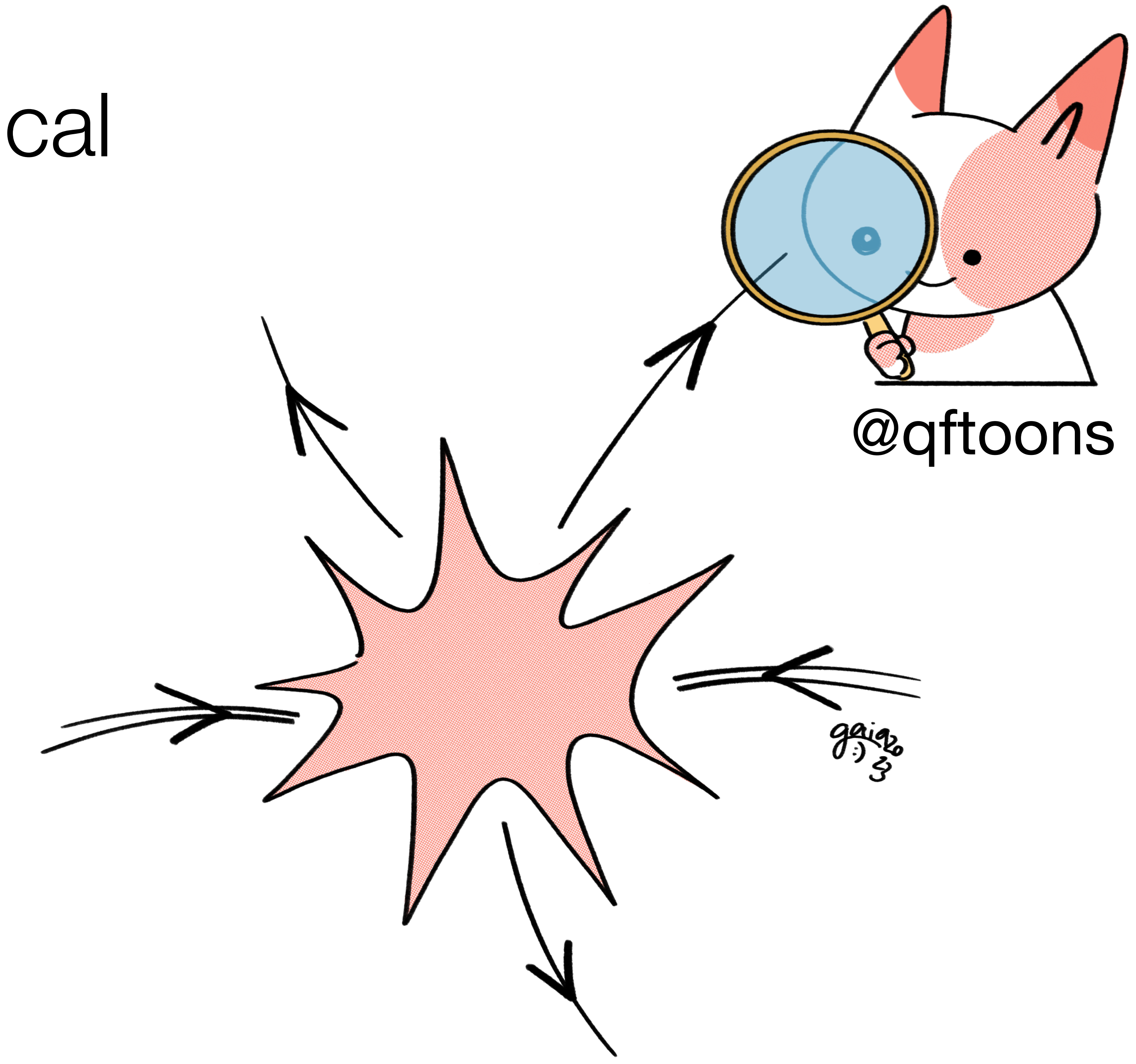
$pp \to \gamma + 2j$ *[Badger, Czakon, Bayu Hartanto, Moodie, Peraro, Poncelet, **SZ** 2023]*

All massless 2→3 processes now analysed at NNLO QCD ✔

Conclusions

New algorithm to construct solutions to canonical DEs using numerical boundary values

- Clear analytic structure
- Efficient computation of amplitudes
- Efficient numerical evaluation



All 2-loop 5-pt integrals with 1 external massive leg now available!

Conclusions

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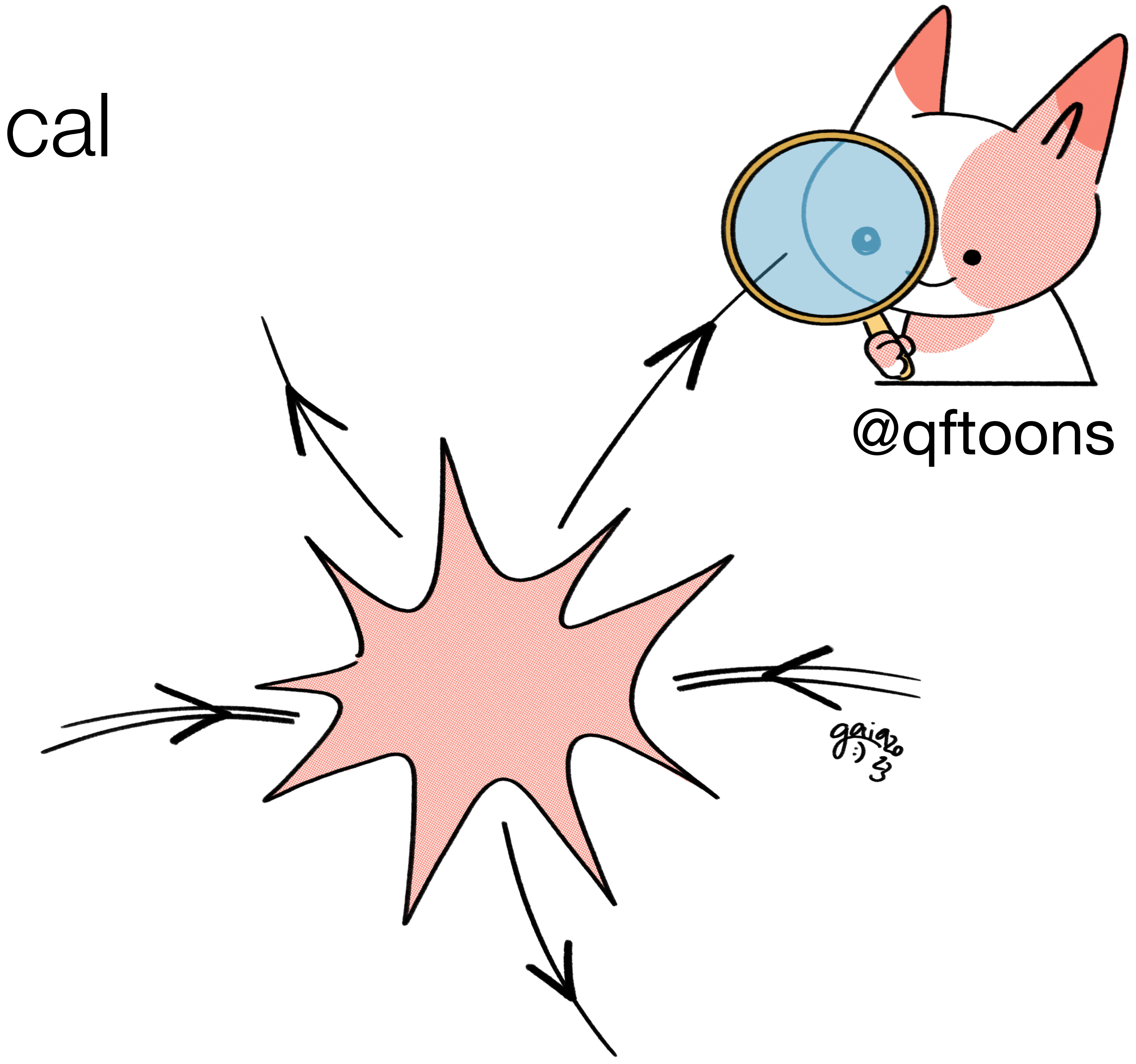
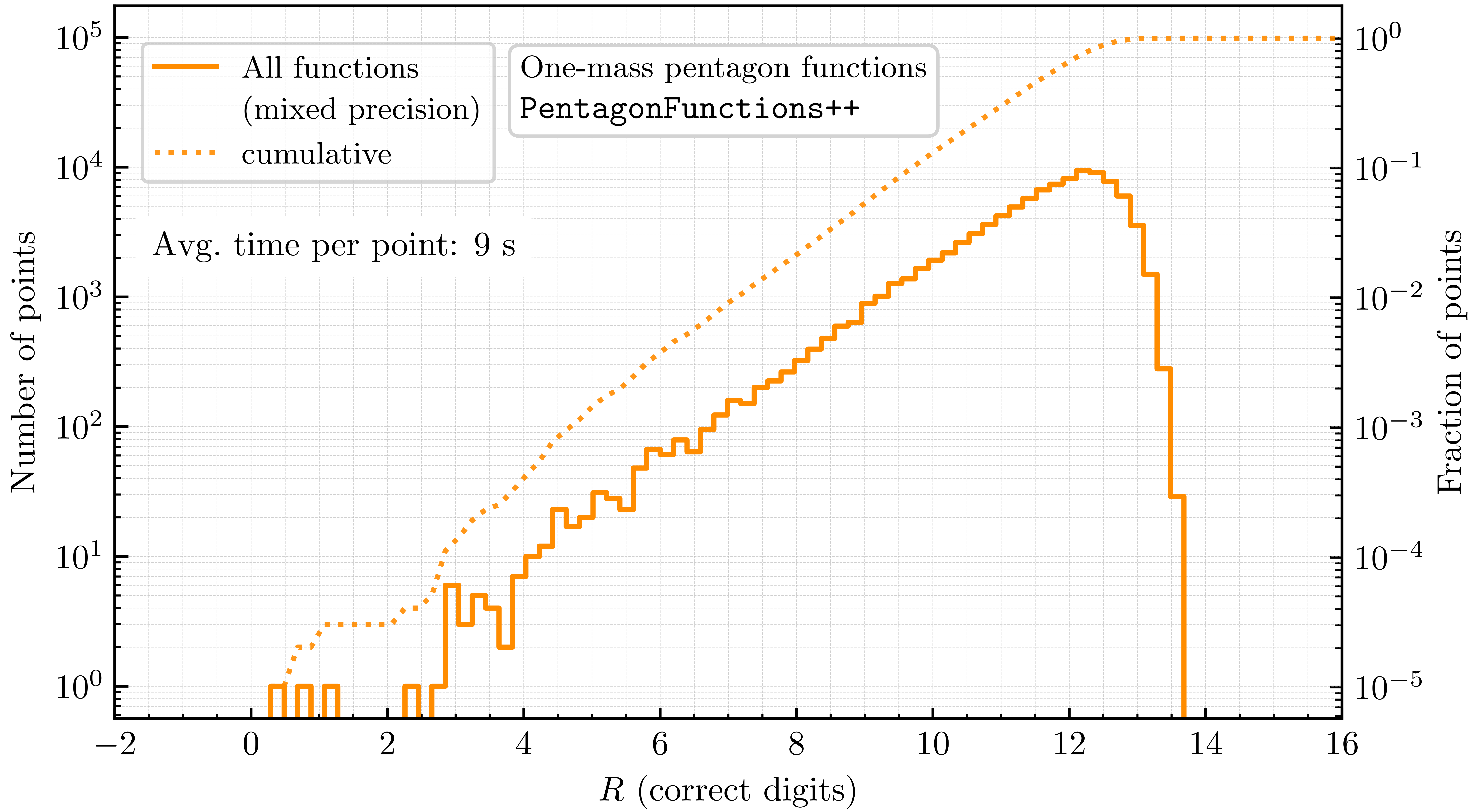


All 2-loop 5-pt integrals with 1 external massive leg now available!

Thank you!



All functions
(mixed precision)
cumulative
One-mass pentagon functions
PentagonFunctions++
Avg. time per point: 9 s
10^5
10^4
10^3
10^2
10^1
10^0
Number of points
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
Fraction of points
−2
0
2
4
6
8
10
12
14
16
R (correct digits)

Solving the canonical DEs in terms of iterated integrals is straightforward

$$\begin{cases} \mathrm{d}\left[w_{i_1}, \ldots, w_{i_n}\right]_{s_0}(s) = \mathrm{d}\log w_{i_n}(s) \left[w_{i_1}, \ldots, w_{i_{n-1}}\right]_{s_0}(s) \\ \left[w_{i_1}, \ldots, w_{i_n}\right]_{s_0}(s_0) = 0 \end{cases}$$

Chen's iterated integrals

Canonical DEs

$$\begin{cases} \mathrm{d}\, \overrightarrow{\mathrm{MI}}^{(w)}(s) = \sum_i a_i \, \mathrm{d}\log w_i(s) \; \overrightarrow{\mathrm{MI}}^{(w-1)}(s) \\ \overrightarrow{\mathrm{MI}}^{(w)}(s_0) = \overrightarrow{\mathrm{MI}}_0^{(w)} \end{cases}$$

Insensitive to square roots!

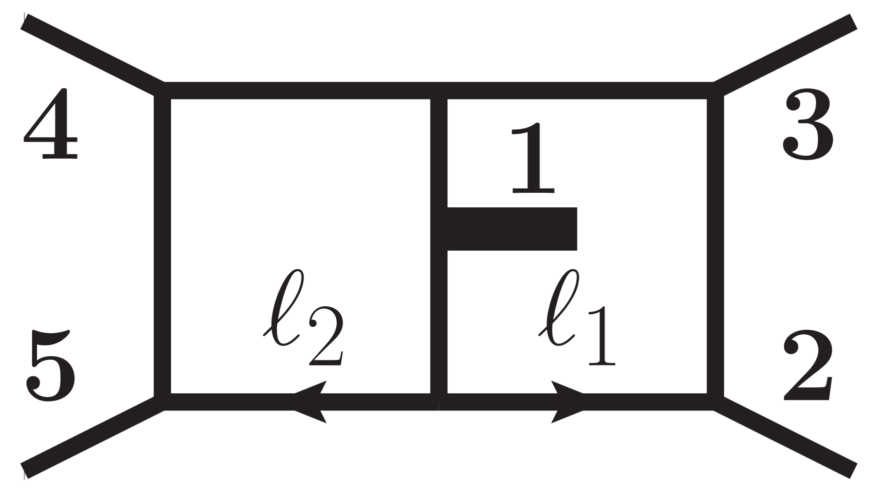
Integral families

$D = 4 - 2\epsilon$

Integer powers

$$\mathrm{I}[\vec{a}](s;\epsilon) = \int \frac{\mathrm{d}^D\ell_1}{\mathrm{i}\pi^{D/2}} \frac{\mathrm{d}^D\ell_2}{\mathrm{i}\pi^{D/2}} \prod_{j=1}^{11} \frac{1}{\rho_j^{a_j}}$$

$s = \{p_1^2, s_{12}, s_{23}, s_{34}, s_{45}, s_{51}\}$ $\quad s_{ij} = (p_i + p_j)^2$



$\rho_1 = \ell_1^2$

$\rho_2 = (\ell_1 + p_2)^2$

$\ldots$

Infinitely many integrals

Infinitely many linear relations

→ Finitely many are linearly independent: the **master integrals**: $\overrightarrow{\mathrm{MI}}$

Integration-by-parts identities (IBPs)

[Tkachov '81; Chetyrkin, Tkachov '81; Laporta 2000]

$$\mathrm{I} = \sum_i c_i \times \mathrm{MI}_i$$