Some optimization aspects related to the numerical evaluation of Master Integrals

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Outline

- Numerical evaluation of Master Integrals expressed as Goncharov Multiple polylogarithms (GPs)

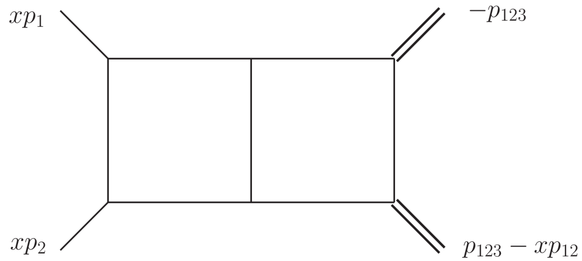
Timing and optimization

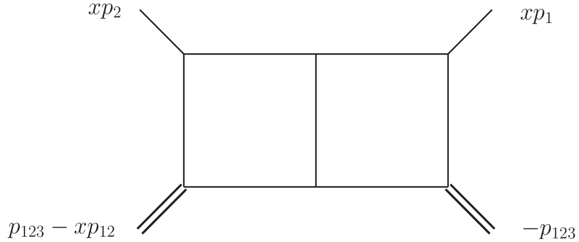
- List-Multiple polylogarithms (L)

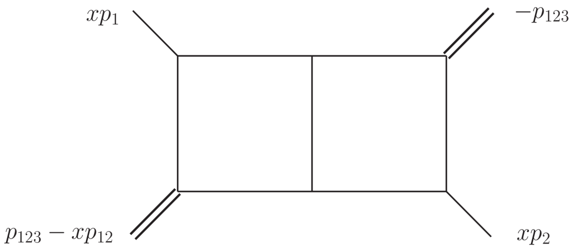
Proposal for a shorter notation for large expressions

Planar double boxes

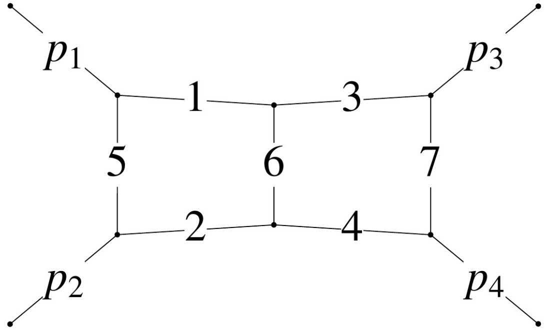
- x-parametrization [Costas G. Papadopoulos, DT, Christopher Wever '14]







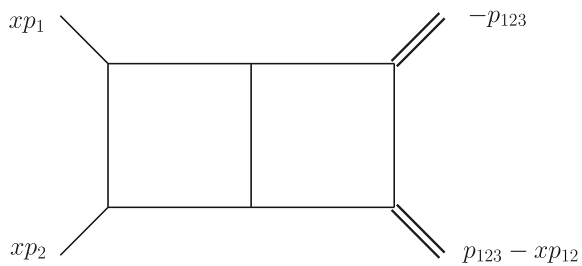
- xyz-parameterization [J. M. Henn, K. Melnikov, and V. A. Smirnov '14]



Planar double boxes

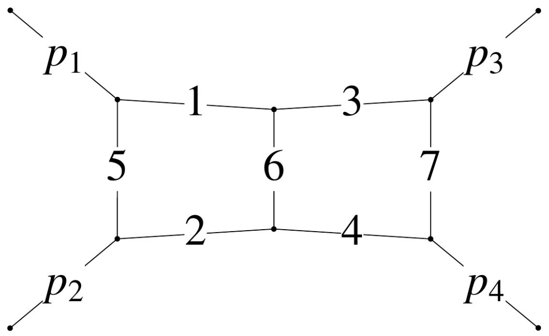
$$S = (q_1 + q_2)^2 = (q_3 + q_4)^2, \quad T = (q_1 - q_3)^2 = (q_2 - q_4)^2$$
$$U = (q_1 - q_4)^2 = (q_2 - q_3)^2, \qquad q_3^2 = M_3^2, q_4^2 = M_4^2$$

- x-parametrization [C. G. Papadopoulos, DT, C. Wever '14]



$$q_1 = xp_1, \quad q_2 = xp_2, \quad q_3 = p_{123} - xp_{12}, \quad q_4 = p_{123},$$
$$p_i^2 = 0, \qquad s_{12} := p_{12}^2, \qquad s_{23} := p_{23}^2, \qquad q := p_{123}^2,$$
$$S = s_{12}x^2, \qquad T = q - (s_{12} + s_{23})x,$$
$$M_3^2 = (1 - x)(q - s_{12}x), \qquad M_4^2 = q$$

- xyz-parameterization [J. M. Henn, K. Melnikov, and V. A. Smirnov '14]



$$\mathrm{P12}: \; p_1 = -q_3, \; p_2 = -q_4, \; p_3 = q_1, \; p_4 = q_2$$
$$\mathrm{P13}: \; p_1 = -q_3, \; p_2 = q_1, \; p_3 = -q_4, \; p_4 = q_2$$
$$\mathrm{P23}: \; p_1 = q_2, \; p_2 = -q_4, \; p_3 = -q_3, \; p_4 = q_1$$
$$\frac{S}{M_3^2} = (1 + \bar{x})(1 + \bar{x}\bar{y}), \quad \frac{T}{M_3^2} = -\bar{x}\bar{z}, \quad \frac{M_4^2}{M_3^2} = \bar{x}^2\bar{y}$$

Planar double boxes

- The two parameterizations are different, but they describe the same physics
- Example: mapping valid for $q<s12$

P12-P13:

$$\bar{x} = -1 + (s12x)/q$$

$$\bar{y} = (q - qx)/(q - s12x)$$

$$\bar{z} = (q - qx + s23x)/(q - s12x)$$

P23:

$$\bar{x} = -1 + (s12x)/q$$

$$\bar{y} = (q - qx)/(q - s12x)$$

$$\bar{z} = (q - (s12 + s23)x)/(q - s12x)$$

Planar double boxes

- Different parameterizations, different solution strategies ⟹ analytic results looks differently (clearly they are equivalent)
- Sample of results for P12, as function of GPs

$$G[1,x]\left(G\left[\frac{s12+s23}{s12},x\right]\left(-\frac{G\left[0,\frac{q}{s12},x\right]}{s12^2}+\frac{G\left[0,\frac{q}{q-s23},x\right]}{s12^2}\right)+G\left[0,1-\frac{s23}{q}\right]\left(-\frac{36\,G\left[0,\frac{q}{s12},x\right]}{s12^2}-\frac{36\,G\left[\frac{q}{s12},\frac{q}{q-s23},x\right]}{s12^2}+\frac{6\,G\left[\frac{q}{s12},\frac{s12+s23}{s12},x\right]}{s12^2}\right)+\ldots\right.$$

x-parametrization

$$G[-1,x]\,(i\pi-G[0,y]+2\,G[0,z])+i\pi\,G\left[-\frac{1}{y},x\right]-i\pi\,G\left[-\frac{1}{z},x\right]+G[0,z]\left(2\,G\left[-\frac{1}{y},x\right]-G\left[-\frac{1}{z},x\right]-G\left[-\frac{z}{y},x\right]\right)-\ldots$$

xyz-parametrization

Planar double boxes

- Comparison of computational time:

$$Phys1 \quad = \quad q \to 3,\ s_{12} \to 14/3,\ s_{23} \to -(5/9),\ x \to 11/10$$

Table 1: P12

MI	Phys1(sec.)
G111010111(x)	3
G111010111(xyz)	< 1
G111m10111(x)	3
G111m10111(xyz)	1
G11101m111(x)	3
G11101m111(xyz)	< 1

Table 2: P13

MI	Phys1(sec.)
G011111011(x)	27
G011111011(xyz)	1
Gm11111011(x)	27
Gm11111011(xyz)	1

Table 3: P23

MI	Phys1(sec.)
G111010111(x)	4
G111010111(xyz)	1
G111m10111(x)	3
G11101m111(xyz)	1

Planar double boxes

- Comparison of computational time:

$$
\begin{aligned}
Phys1 &= q \to 3,\ s_{12} \to 14/3,\ s_{23} \to -(5/9),\ x \to 11/10 \\
Phys2 &= q \to 7/3,\ s_{12} \to 30/4,\ s_{23} \to -(5/2),\ x \to 11/2
\end{aligned}
$$

Table 1: P12

MI	Phys1(sec.)	Phys2(sec.)
G111010111(x)	3	1
G111010111(xyz)	<1	11
G111m10111(x)	3	2
G111m10111(xyz)	1	17
G11101m111(x)	3	2
G11101m111(xyz)	<1	8

Table 2: P13

MI	Phys1(sec.)	Phys2(sec.)
G011111011(x)	27	7
G011111011(xyz)	1	15
Gm11111011(x)	27	7
Gm11111011(xyz)	1	15

Table 3: P23

MI	Phys1(sec.)	Phys2(sec.)
G111010111(x)	4	2
G111010111(xyz)	1	8
G111m10111(x)	3	2
G11101m111(xyz)	1	9

Large differences in computational costs!

GPs evaluation

- Definition $$G(z_1,\dots,z_k;y) \;=\; \int_0^y \frac{dt_1}{t_1-z_1}\int_0^{t_1}\frac{dt_2}{t_2-z_2}\dots\int_0^{t_{k-1}}\frac{dt_k}{t_k-z_k}.$$
- Evaluation: algorithm dependent on the input values

[J. Vollinga, S. Weinzierl '04]

- $|y| \le |z_j|$ for all j $\quad y/z_1 \neq 1$

$$G(z_1,\dots,z_k;y) = \sum_{j_1=1}^{\infty}\dots\sum_{j_k=1}^{\infty}\frac{1}{j_1+\dots+j_k}\left(\frac{y}{z_1}\right)^{j_1}\frac{1}{j_2+\dots+j_k}\left(\frac{y}{z_2}\right)^{j_2}\dots\frac{1}{j_k}\left(\frac{y}{z_k}\right)^{j_k}$$

- if $|y| > |z|$ $\quad G(z,y) = G(y,z) - G(0,z) + I\pi G(0,y)$

  in general if $|y| > |z_i|$ $\quad G(\dots z_i \dots, y) = \sum(\dots)G(\dots)$

- slow convergence if |y/z|~1 (Holder convolution or other strategies)

$$G(z_1,\dots,z_w;1) \;=\; \sum_{j=0}^{w}(-1)^j G\left(1-z_j,1-z_{j-1},\dots,1-z_1;1-\frac{1}{p}\right)G\left(z_{j+1},\dots,z_w;\frac{1}{p}\right)$$

GPs evaluation

- Definition $$G(z_1,\ldots,z_k;y) = \int_0^y \frac{dt_1}{t_1-z_1}\int_0^{t_1}\frac{dt_2}{t_2-z_2}\ldots\int_0^{t_{k-1}}\frac{dt_k}{t_k-z_k}.$$
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- if $|y| > |z|$ $\quad G(z,y) = G(y,z) - G(0,z) + I\pi G(0,y)$

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"Fast" $G(1,2,3;0.001) \to 5\cdot 10^{-4}$sec. $\quad$ "Slow" $G(1,2,3;1.999) \to 4\cdot 10^{-2}$sec.

Main message

- Once we have analytic solution for some MI we prefer to simplify it in order to achieve a fast evaluation
- It is NOT obvious what is the best expression, not always expression made of few GPs is the fastest expression to be evaluated.
- MAYBE: according to different regions and limits in the phase space, there could be differently optimized expressions ⇒ $\mathrm{fibrationBasis()}$ in $\mathrm{Hyperint}$ code can be useful for this scope

[E. Panzer '15]

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  [E. Panzer '15]

- Simplification must take into account numerical evaluation features of GPs functions

List-GPs proposal

- Master integrals expressed as sum of several GPs. For MI with 7 propagators ~10^5
- Proliferation of terms coming from partial fractioning procedure

$$\int_0^x \frac{dt}{(t-a_1)(t-a_2)(t-a_3)} = \frac{G(a_1;x)}{(a_1-a_2)(a_1-a_3)} + \frac{G(a_2;x)}{(a_2-a_1)(a_2-a_3)} + \frac{G(a_3;x)}{(a_3-a_1)(a_3-a_2)}$$

$$\int_0^x \frac{dt_1}{(t_1-a_1)(t_1-a_2)(t_1-a_3)} \int_0^{t_1} \frac{dt_2}{(t_2-b_1)(t_2-b_2)(t_2-b_3)(t_2-b_4)} = \sum (12\text{GPs})$$

- We may introduce a compact notation

$$\int_0^x \frac{dt_1}{(t_1-a_1)(t_1-a_2)(t_1-a_3)} \int_0^{t_1} \frac{dt_2}{(t_2-b_1)(t_2-b_2)(t_2-b_3)(t_2-b_4)} \equiv L\left(\left\{\begin{array}{c} a_1 \\ a_2 \\ a_3 \end{array}\right\}, \left\{\begin{array}{c} b_1 \\ b_2 \\ b_3 \\ b_4 \end{array}\right\}; x\right)$$

$$\int_0^x \frac{dt_1}{t_1(t_1-a_2)(t_1-a_3)} \int_0^{t_1} \frac{dt_2}{(t_2-b_1)(t_2-b_2)^2} \equiv L\left(\left\{\begin{array}{c} 0 \\ a_2 \\ a_3 \end{array}\right\}, \left\{\begin{array}{c} b_1 \\ b_2 \\ b_2 \end{array}\right\}; x\right)$$

List-GPs definition

$$L(\bar{a}_k, \bar{a}_{k-1} \ldots \bar{a}_2, \bar{a}_1, x) \equiv$$
$$\int_0^x \frac{dt_k}{\prod_{i_k=1}^{n_k}(t_k - a_{i_k})} \int_0^{t_k} \frac{dt_{k-1}}{\prod_{i_{k-1}=1}^{n_{k-1}}(t_{k-1} - a_{i_{k-1}})} \int_0^{t_{k-1}} \cdots \int_0^{t_3} \frac{dt_2}{\prod_{i_2=1}^{n_2}(t_2 - a_{i_2})} \int_0^{t_2} \frac{dt_1}{\prod_{i_1=1}^{n_1}(t_1 - a_{i_1})}$$

$$\bar{a}_i \equiv \{a_{i_1}, a_{i_2} \ldots, a_{i_n}\}$$

- L is a linear combination of G.
- In some cases we can write explicit formula.

If $a_{i_j} \neq a_{i_k}$ for each $a_i \Rightarrow$

$$L(\bar{a}_k, \bar{a}_{k-1} \ldots \bar{a}_2, \bar{a}_1, x) = \sum_{i_k, i_{k-1}, \ldots, i_2, i_1=1}^{n_k, n_{k-1}, \ldots, n_2, n_1} \left(\frac{1}{P(\bar{a}_k, i_k) P(\bar{a}_{k-1}, i_{k-1}) \ldots P(\bar{a}_1, i_1)} \right) G(a_{i_k} \ldots a_{i_1}, x)$$

$$P(\bar{a}_k, i) = \prod_{j=1, j \neq i}^{n} (a_{k_i} - a_{k_j})$$

Shuffle algebra

- L functions satisfies shuffle algebra.
- In simple cases, it can be directly verified by using explicit GPs representation

$$L(\bar{a}_1, x)L(\bar{a}_2, x) = \left(\sum_{i_1} \frac{G(a_{i_1}, x)}{P(\bar{a}_1, i_1)}\right) \cdot \left(\sum_{i_2} \frac{G(a_{i_2}, x)}{P(\bar{a}_2, i_2)}\right) =$$

$$= \left(\sum_{i_1, i_2} \frac{G(a_{i_1}, a_{i_2}, x) + G(a_{i_2}, a_{i_1}, x)}{P(\bar{a}_1, i_1) \cdot P(\bar{a}_2, i_2)}\right) = L(\bar{a}_1, \bar{a}_2, x) + L(\bar{a}_2, \bar{a}_1, x)$$

- In general shuffle is property of nested integrations (valid if pathologic integrands are avoided)

$$L(\bar{a}_1, x)L(\bar{a}_2, x) = L(\bar{a}_1, \bar{a}_2, x) + L(\bar{a}_2, \bar{a}_1, x)$$

[Numerical and Symbolic Scientific Computing, Langer-Paule & references there's in]

L functions and MI

- Using L notation the result of MI can be more compact and manageable.
- A direct numerical evaluation of L may speed-up the MI evaluation (instead of expanding L in sum of G and then evaluate all of them separately)
- In principle a further generalization to any rational integrand is possible, but it is not obvious whether will provide benefit for the MI applications:

$$L(\bar{a}_k, \bar{a}_{k-1} \ldots \bar{a}_2, \bar{a}_1, x) \equiv$$

$$\int_0^x dt_k \frac{\prod_{j_k=1}^{m_k}(t_k - \alpha_{j_k})}{\prod_{i_k=1}^{n_k}(t_k - a_{i_k})} \int_0^{t_k} dt_{k-1} \frac{\prod_{j_{k-1}=1}^{m_{k-1}}(t_{k-1} - \alpha_{j_{k-1}})}{\prod_{i_{k-1}=1}^{n_{k-1}}(t_{k-1} - a_{i_{k-1}})} \int_0^{t_{k-1}} \ldots \int_0^{t_2} dt_1 \frac{\prod_{j_1=1}^{m_1}(t_1 - \alpha_{j_1})}{\prod_{i_1=1}^{n_1}(t_1 - a_{i_1})}$$

$$\bar{a}_i \equiv \{\{\alpha_{j_1}, \alpha_{j_2} \ldots, \alpha_{j_m}\}, \{a_{i_1}, a_{i_2} \ldots, a_{i_n}\}\}$$

Summary

- Not all the needed two-loop Master Integrals are known yet, but it is already time to start thinking how to make a library of them
- In particular it is important trying to understand how to simplify them, but first of all we must understand what does it mean: “simplified”
- Maybe some more general functions than Goncharov Multiple polylogarithms are suitable for this task

Thanks!