Numerical calculations in $d = 4$

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Outline

1. Introduction: three bottlenecks in NN(N)LO calculations

2. Towards “the” 4-dimensional numerical approach

3. (Personal) outlook
Very active field!

- Z. Capatti, V. Hirschi, D. Kermanschah, A. Pelloni, B. Ruijl [1912.09291, 1906.06138]
- F. Driencourt-Mangin, G. Rodrigo, G. Sborlini, W. Torres [1911.11125]
- V. Del Duca, N. Deutschmann, S. Lionetti [1910.01024]
- C. Anastasiou, G. Sterman [1812.03753]
- B. Page, R.P. [1810.00234]
- F. Herzog [1804.07949]
The LO past to understand the $N^3$LO present

Why high-multiplicity ($n_p \sim 10$) LO perturbative calculations are nowadays the bread and butter of high-energy particle physics simulations?

i) 4 dimensions

ii) No UV/IR divergences

iii) No contour deformation to compute integrals

Take, for instance,

$$\sigma_{n_p=10}^{\text{cut}} := \int_{\text{cut}} d\Phi_{10} |M|^2$$

Nobody would ever try to compute $\sigma_{n_p=10}^{\text{cut}}$ analytically.

Due to i), ii), iii), Monte Carlo methods can be used to find a numerical approximation of $\sigma_{n_p=10}^{\text{cut}}$. 
The ultimate solution in multiloop calculations

A **direct** Monte Carlo integration over both loop functions and phase-space integrals

- Any numerical method aiming at this must obey i), ii), iii)
- In what follows, I discuss the current achievements towards i), ii), iii) of

i) 4 dimensions

ii) No UV/IR divergences
UV in 4 dimensions

\[ I^1 = \int d^4 q \frac{1}{(q^2 - M^2)^2} = ? \]

The UV divergent part is extracted via partial fractioning \((q^2 \to \bar{q}^2 := q^2 - \mu^2)\)

\[ \frac{1}{(\bar{q}^2 - M^2)^2} = \frac{1}{\bar{q}^4} + \left( \frac{M^2}{\bar{q}^2(\bar{q}^2 - M^2)^2} + \frac{M^2}{\bar{q}^4(\bar{q}^2 - M^2)} \right) \]

The “problematic” piece is

- Fixed by QFT symmetries [IREG]
- Used to build integrand-level DReg UV counterterms for a local UV subtraction [FDU]
- Dropped [FDR]
FDR integrals

\[ I_{\text{FDR}}^1 = \int [d^4 q] \frac{1}{(q^2 - M^2)^2} = -i\pi^2 \ln \frac{M^2}{\mu_R^2} \]

\[ \text{FDR integral} \quad \text{Renormalization scale} \]

Regularization and Renormalization at once

- It can be generalized to more loops

\[ I_{\text{FDR}}^\ell = \sum_{k=0}^{\ell} c_k \ln^k (\mu_R^2) \]

- **No UV divergences** when computing loop integrals, e.g.

\[ I_{\text{FDR}}^1 = \int d^4 q \left[ \frac{1}{(q^2 - M^2)^2} - \frac{1}{(q^2 - \mu_R^2)^2} \right] \]
Two QFT core tenets respected by FDR

1. **Gauge invariance**
   - FDR integrals are invariant under the shift $q \rightarrow q + p \ \forall p$
   - Cancellations between numerators and propagators

$$\int [d^4 q] \frac{q^2}{q^2 (q^2 - M^2)^2} = \int [d^4 q] \frac{1}{(q^2 - M^2)^2}$$

$\Rightarrow$ One can prove graphical WI in QFT

2. **Unitarity of $S = I + iT$**

$$\Rightarrow \ i(T - T^\dagger) = -T^\dagger T \ \text{can be enforced}$$
The fate of $\mu_R$ in FDR

Given $\mathcal{L}(p_1, \ldots, p_m)$ and

$$\tilde{p}_k(\mu_R) := p_k^{\text{TH,}\ell-\text{loop}}(O_1^{\text{EXP}}, \ldots, O_m^{\text{EXP}}, \mu_R) \quad (k = 1 \div m)$$

- Renormalizable Lagrangian:

$$\frac{dO_{m+1}^{\text{TH,}\ell-\text{loop}}(\tilde{p}_1(\mu_R), \ldots, \tilde{p}_m(\mu_R), \mu_R)}{d\mu_R} = 0$$

No $\mathcal{L} = \mathcal{L}_R + \Delta \mathcal{L}$ Couterterms

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Numerical calculations in $d = 4$
IR in 4 dimensions

- LTD transforms loop diagrams of $\sigma_V$ into trees which act as local counterterms in PS integrals of $\sigma_R$ [FDU]

  $\Rightarrow$ fully numerical computation in $d = 4$

- The replacement $q^2 \rightarrow q^2 - \mu^2$ regulates in $d = 4$ IR divergences of $\sigma_V$. $\ln \mu^2$ terms cancel in $\sigma_V + \sigma_R$ [FDR]

A systematic local cancellation is not yet available in FDR, but explicit calculations show that $\sigma_V + \sigma_R$ is right up to NNLO

- In both FDU and FDR the key observation is part of $\sigma_V$ should be moved to $\sigma_R$. E.g.

$$\int d\Phi_2 \Re \left( \int [d^4 q] \frac{1}{\bar{q}^2 \bar{D}_1 \bar{D}_2} \right) = \int d\bar{\Phi}_3 \frac{1}{s_{13} s_{23}}$$

- ISR under study
\( H \rightarrow \gamma\gamma \) at two loops in LTD/FDU


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Numerical calculations in \( d = 4 \)
NNLO final-state quark-pair corrections in FDR


\[ A_{n,IR}^{(2)} = \int d\Phi_n \sum_{\text{spin}} |A_n^{(0)}|^2 \]

\[ \sigma_B \propto \int d\Phi_n \sum_{\text{spin}} |A_n^{(0)}|^2 \]

\[ \sigma_V \propto \int d\Phi_n \sum_{\text{spin}} \left\{ A_n^{(2)}(A_n^{(0)})^* + A_n^{(0)}(A_n^{(2)})^* \right\} \]

\[ \sigma_R \propto \int d\Phi_{n+2} \sum_{\text{spin}} \left\{ A_{n+2}^{(0)}(A_{n+2}^{(0)})^* \right\} \]

\[ \sigma_{\text{NNLO}} = \sigma_B + \sigma_V + \sigma_R \]
Known IR finite results reproduced by FDR

\[ H \to b\bar{b} + jets \]

\[
\Gamma^{\text{NNLO}}_{\gamma^* \to jets} = \Gamma_2^{(0)} (y_b) \left\{ 1 + a^2 C_F N_F \left( 2 \ln^2 \frac{m_b^2}{M_H^2} - \frac{26}{3} \ln \frac{m_b^2}{M_H^2} + 8\zeta_3 + 2\pi^2 - \frac{62}{3} \right) \right\}
\]

\[
\sigma^{\text{NNLO}}_{e^+e^- \to jets} = \sigma_2^{(0)} \left\{ 1 + a^2 C_F N_F (8\zeta_3 - 11) \right\}
\]

\[
a = \frac{\alpha_s}{4\pi}
\]
iii)

No contour deformation to compute integrals
A toy model of the problem

In the phase space (positive definite integrands):

\[ I_{PD} = \int_{0.5}^{1} dx \frac{\sqrt{3x^3 + 2x^2 + x + 1}}{x} = 1.380(1) \]

In the loop functions (threshold singularities):

\[ I_{NPD} = \int_{-1}^{1} dx \frac{\sqrt{3x^3 + 2x^2 + x + 1 + i\epsilon}}{x + i\epsilon} = ? \]

To compute \( I_{NPD} \) numerically one can use:
- contour deformation (not too much, not to cross the branch cut of the square root)
- Sokhotski–Plemelj (to extract the singularity at \( x = 0 \))

Both solutions require analytical work

No direct MC integration
A direct MC integration is possible

\[ I_{\text{NPD}} = \int_{-1}^{1} dx \frac{\sqrt{3x^3 + 2x^2 + x + 1 + i\epsilon}}{x + i\epsilon} = 1.696(1) - i3.291(1) \]

- MC error of the same order of the PD case
- Any 4-dimensional method can implement this
- Any integrand is allowed, e.g.

\[ \int_{-1}^{1} dx \frac{\ln(x - \sqrt{x^2 - 2x - 1 + i\epsilon - i\epsilon})}{x + i\epsilon} = -3.939(1) + i2.752(2) \]

- Applying this to multiloop functions renders reduction methods to MI obsolete
The roadmap towards a fully numerical treatment of \texttt{NN(N)LO} computations is (surprisingly!) clear.

The three main ingredients
- $d=4$
- reshuffling contributions to avoid UV/IR divergences
- MC integration over non positive definite integrands

are in place and we have ideas on how to mount them to produce realistic perturbative predictions.

My (personal) estimate to achieve a general working algorithm at the \texttt{NNLO}:

5-6 years

assuming people with 100\% dedication to this

\texttt{N^3LO at reach} before the start of the FCC.
Thanks!
Backup slides
"Vacuum" subtraction

1. \( J(q^2) = \frac{1}{(q^2 - M^2)^2} \)
2. \( q^2 \xrightarrow{\text{GP}} \bar{q}^2 := q^2 - \mu^2 \)
3. \( J(q^2) \xrightarrow{\text{GP}} \bar{J}(\bar{q}^2) := \frac{1}{(\bar{q}^2 - M^2)^2} \)

\[
\frac{1}{(\bar{q}^2 - M^2)^2} = \left[ \frac{1}{\bar{q}^4} \right] + \left( \frac{M^2}{\bar{q}^2(\bar{q}^2 - M^2)^2} + \frac{M^2}{\bar{q}^4(\bar{q}^2 - M^2)} \right)
\]

Vacuum
**“Vacuum” subtraction**

1. \( J(q^2) = \frac{1}{(q^2 - M^2)^2} \)

2. \( q^2 \xrightarrow{\text{GP}} \bar{q}^2 := q^2 - \mu^2 \)

3. \( J(q^2) \xrightarrow{\text{GP}} \bar{J}(\bar{q}^2) := \frac{1}{(\bar{q}^2 - M^2)^2} \)

\[
\frac{1}{(\bar{q}^2 - M^2)^2} = \left[ \frac{1}{\bar{q}^4} \right] + \left( \frac{M^2}{\bar{q}^2(\bar{q}^2 - M^2)^2} + \frac{M^2}{\bar{q}^4(\bar{q}^2 - M^2)} \right)
\]

\[
\int \left[ d^4 q \right] \frac{1}{(\bar{q}^2 - M^2)^2} := \lim_{\mu \to 0} \int d^4 q \left( \frac{M^2}{\bar{q}^2(\bar{q}^2 - M^2)^2} + \frac{M^2}{\bar{q}^4(\bar{q}^2 - M^2)} \right)
\]

and \( \mu = \mu_R \) after the asymptotic \( \mu \to 0 \) limit
Examples of two-loop vacua

- **Global vacua** \((q_{12} := q_1 + q_2)\):

\[
\begin{bmatrix}
\frac{1}{\bar{q}_1^2 \bar{q}_2^2 \bar{q}_{12}^2} \\
\bar{q}_1^4 \bar{q}_2^2 \bar{q}_{12}^2
\end{bmatrix},
\begin{bmatrix}
\frac{1}{\bar{q}_1^4 \bar{q}_2^2 \bar{q}_{12}^2} \\
\bar{q}_1^4 \bar{q}_2^2 \bar{q}_{12}^2
\end{bmatrix},
\begin{bmatrix}
\frac{1}{\bar{q}_1^4} \\
\frac{1}{\bar{q}_2^4}
\end{bmatrix}
\]

- **Sub-vacua:**

\[
\frac{M^4}{(\bar{q}_1^2 - M^2)\bar{q}_1^4} \begin{bmatrix}
1 \\
\frac{1}{\bar{q}_2^2}
\end{bmatrix},
\frac{M^4}{(\bar{q}_1^2 - M^2)^2\bar{q}_1^4} \begin{bmatrix}
1 \\
\frac{1}{\bar{q}_2^2}
\end{bmatrix}
\]
Examples of two-loop vacua

- **Global vacua** \((q_{12} := q_1 + q_2):\)

\[
\begin{bmatrix}
\frac{1}{q_1^2} & \frac{1}{q_2^2} & \frac{1}{q_{12}^2}
\end{bmatrix}, \quad \begin{bmatrix}
\frac{1}{q_1^2} & \frac{1}{q_2^2} & \frac{1}{q_{12}^2}
\end{bmatrix}, \quad \begin{bmatrix}
\frac{1}{q_1^4} & \frac{1}{q_2^4}
\end{bmatrix}
\]

- **Sub-vacua:**

\[
\frac{M^4}{(q_1^2 - M^2) q_1^4} \begin{bmatrix}
\frac{1}{q_2^2}
\end{bmatrix}, \quad \frac{M^4}{(q_1^2 - M^2)^2 q_1^2} \begin{bmatrix}
\frac{1}{q_2^4}
\end{bmatrix}
\]

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A two-loop example

\[
\frac{1}{\bar{D}_1 \bar{D}_2 \bar{D}_{12}} = \left[ \frac{1}{\bar{q}_1^2 \bar{q}_2^2 \bar{q}_{12}^2} \right] - m_i^2 \left[ \frac{1}{\bar{q}_1^2 \bar{q}_2^2 \bar{q}_{12}^2} \right] + m_1^2 \left[ \frac{1}{\bar{q}_1^4 \bar{q}_2^4 \bar{q}_{12}^4} \right] - m_1^4 \frac{q_1^2 + 2(q_1 \cdot q_2)}{(\bar{D}_1 \bar{q}_1^4) \bar{q}_2^4 \bar{q}_{12}^2} + m_2^2 \left[ \frac{1}{\bar{q}_1^2 \bar{q}_2^4 \bar{q}_{12}^2} \right] - m_2^4 \frac{q_2^2 + 2(q_1 \cdot q_2)}{\bar{q}_1^4 (\bar{D}_2 \bar{q}_2^4) \bar{q}_{12}^2} + m_{12}^2 \left[ \frac{1}{\bar{q}_1^2 \bar{q}_2^4 \bar{q}_{12}^4} \right] - m_{12}^4 \frac{q_{12}^2 - 2(q_1 \cdot q_{12})}{\bar{q}_1^4 \bar{q}_2^4 (\bar{D}_{12} \bar{q}_{12}^4)} + m_{12}^2 \frac{m_1^2 m_2^2}{\bar{D}_1 \bar{q}_1^2 (\bar{D}_2 \bar{q}_2^2) \bar{q}_{12}^2} + m_{12}^4 \frac{m_1^2 m_2^2}{\bar{q}_1^2 (\bar{D}_2 \bar{q}_2^2) (\bar{D}_{12} \bar{q}_{12}^2)} + m_{12}^2 \frac{m_1^2 m_2^2}{\bar{D}_1 \bar{q}_1^2 (\bar{D}_2 \bar{q}_2^2) (\bar{D}_{12} \bar{q}_{12}^2)} + m_{12}^4 \frac{m_1^2 m_2^2}{\bar{D}_1 \bar{q}_1^2 (\bar{D}_2 \bar{q}_2^2) (\bar{D}_{12} \bar{q}_{12}^2)} + m_{12}^4 \frac{m_1^2 m_2^2}{\bar{q}_1^2 (\bar{D}_2 \bar{q}_2^2) (\bar{D}_{12} \bar{q}_{12}^2)} + m_{12}^4 \frac{m_1^2 m_2^2}{\bar{D}_1 \bar{q}_1^2 (\bar{D}_2 \bar{q}_2^2) (\bar{D}_{12} \bar{q}_{12}^2)} + \frac{m_1^4}{m_{12}^4} \frac{D_{12} \bar{q}_{12}^2}{D_{12} \bar{q}_{12}^2}
\]

\[
(\bar{D}_i := \bar{q}_i^2 - m_i^2)
\]

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Numerical calculations in \( d = 4 \)
Three-loop logarithmic vacua

\[
\frac{1}{\bar{q}_1^2 \bar{q}_2^2 \bar{q}_3^2 \bar{q}_{12}^2 \bar{q}_{13}^2 ((q_2 - q_3)^2 - \mu^2)}
\]

\[
\begin{bmatrix}
1 \\
\frac{1}{\bar{q}_1^2 \bar{q}_3^2 \bar{q}_2^4 \bar{q}_{12}^2 \bar{q}_{23}^2}
\end{bmatrix}
\]

\[
\begin{bmatrix}
1 \\
\frac{1}{\bar{q}_1^4 \bar{q}_2^2 \bar{q}_3^2 \bar{q}_{12}^2 \bar{q}_{123}^2}
\end{bmatrix}
\]

\[
\begin{bmatrix}
1 \\
\frac{1}{\bar{q}_1^4 \bar{q}_2^4 \bar{q}_3^2 \bar{q}_{123}^2}
\end{bmatrix}
\]

\[
\begin{bmatrix}
1 \\
\frac{1}{\bar{q}_1^6 \bar{q}_2^2 \bar{q}_3^2 \bar{q}_{123}^2}
\end{bmatrix}
\]
Unitarity

In any multi-loop Feynman diagram the divergent sub-diagrams must be treated consistently with the lower loop calculations.