

# Computing Feynman Integrals Numerically & ZH Production via Gluon Fusion

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In collaboration with:

Chen, Heinrich, Kerner, Klappert, Schlenk

+ Jahn, Langer, Magerya, Pöldaru, Villa

+ Davies, Mishima, Steinhauser

TBA [22XX.XXXX]

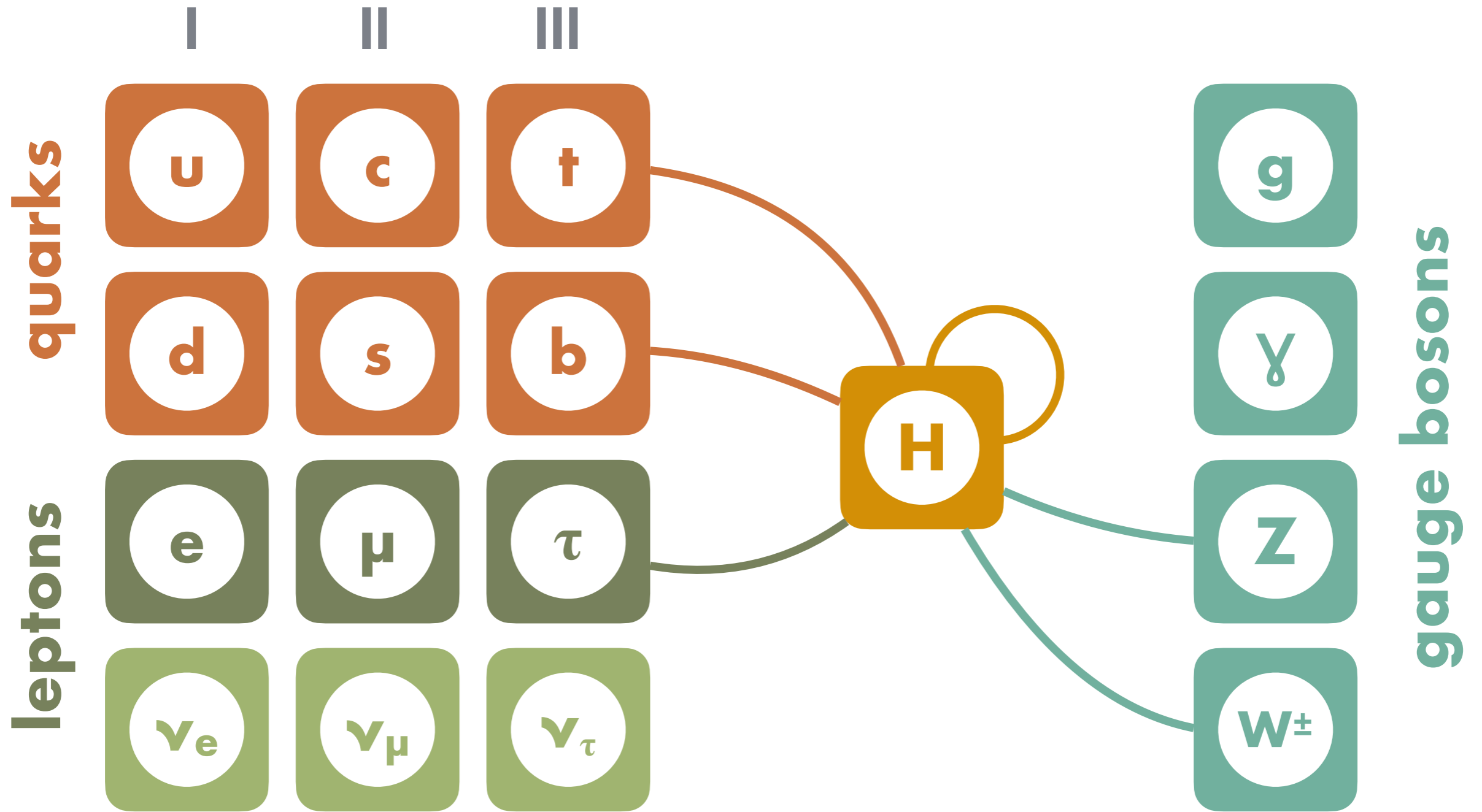
pySecDec Release [2108.10807]

JHEP 03 (2021) 125 [2011.12325]

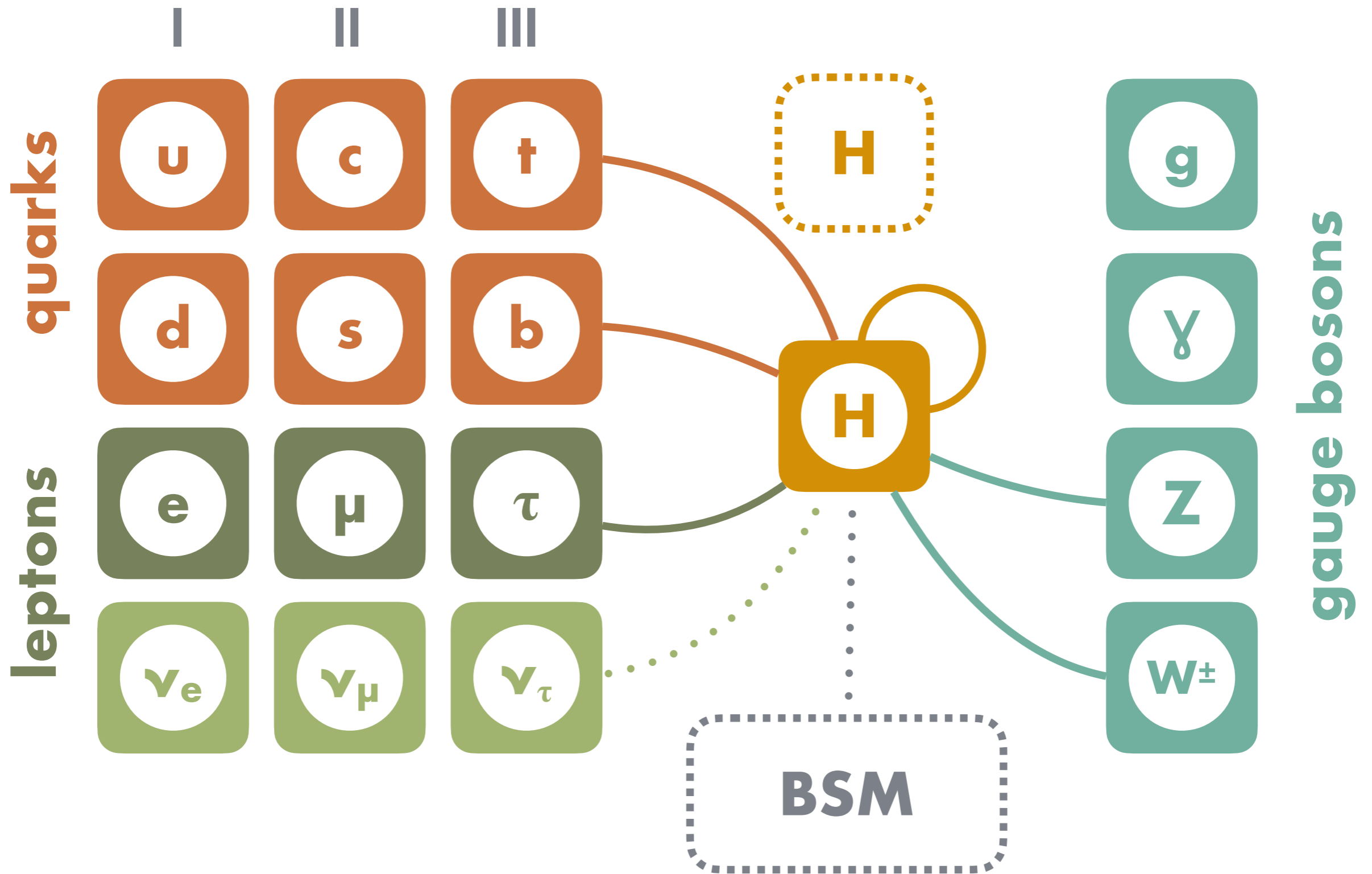


The logo for The Royal Society, consisting of a solid red square with the text "THE ROYAL SOCIETY" in white, all-caps, serif font.

# The Standard Model

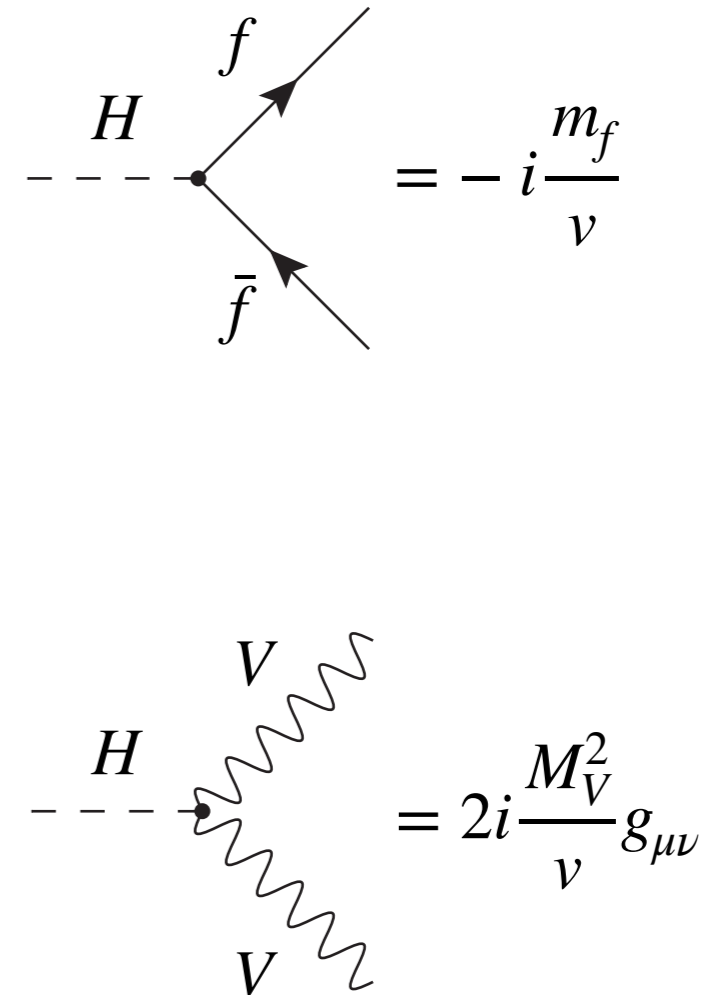
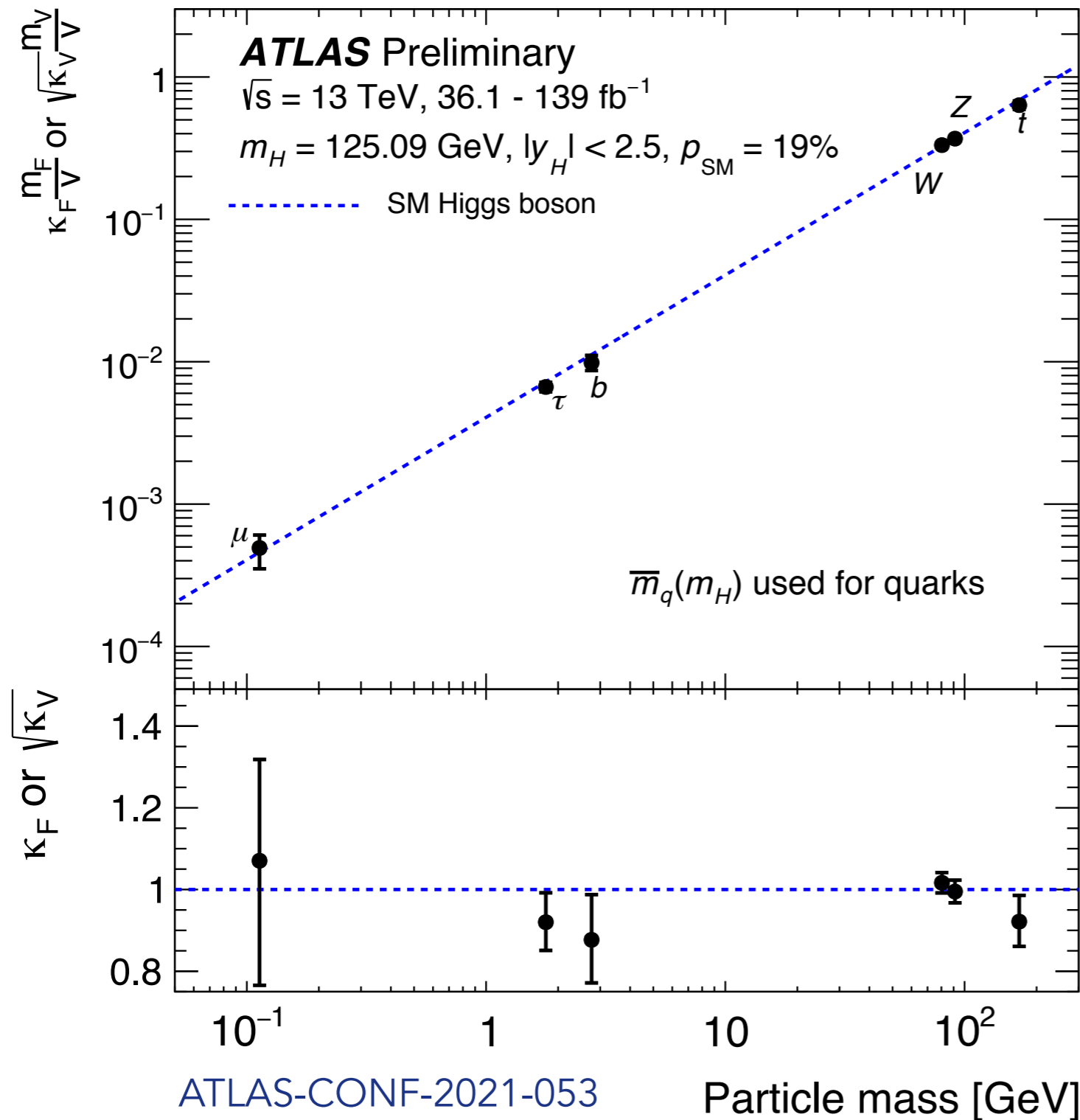


# The Standard Model and Beyond



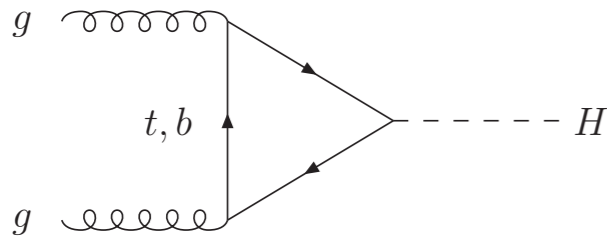
# Higgs Couplings

Incredible progress has been made in establishing properties of the Higgs Boson



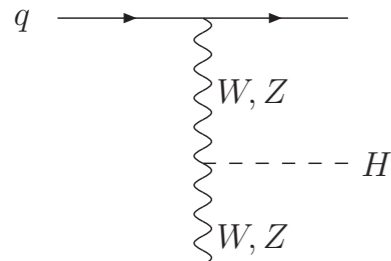


# Higgs Production & Decay

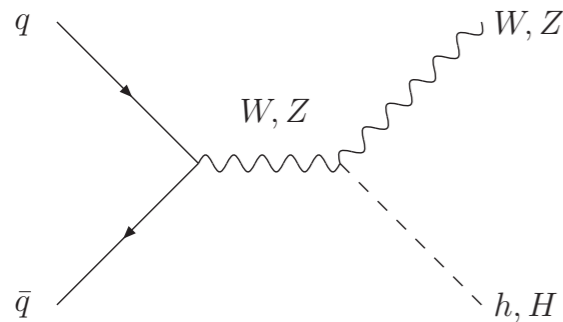


$\sigma$  [pb] @ 13 TeV  
# Higgs in 140 fb<sup>-1</sup>

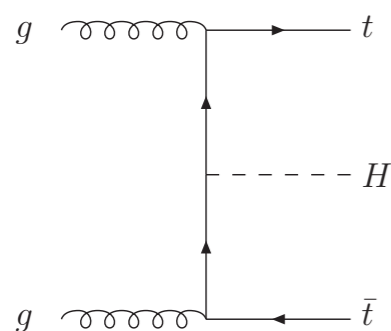
49 pb / 6.9M



3.8 pb / 520k

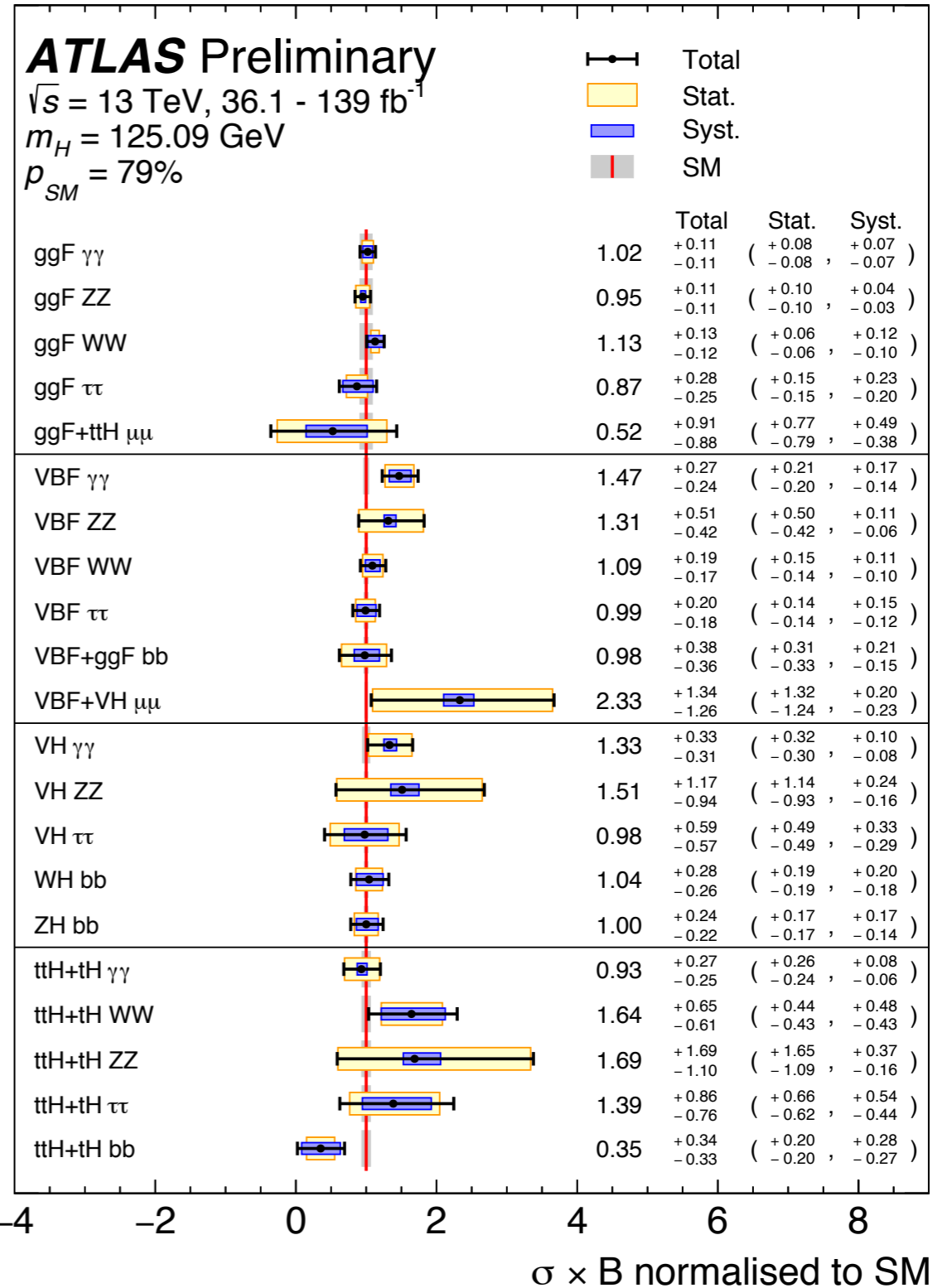


2.3 pb / 320k



0.5 pb / 70k

ATLAS-CONF-2021-053



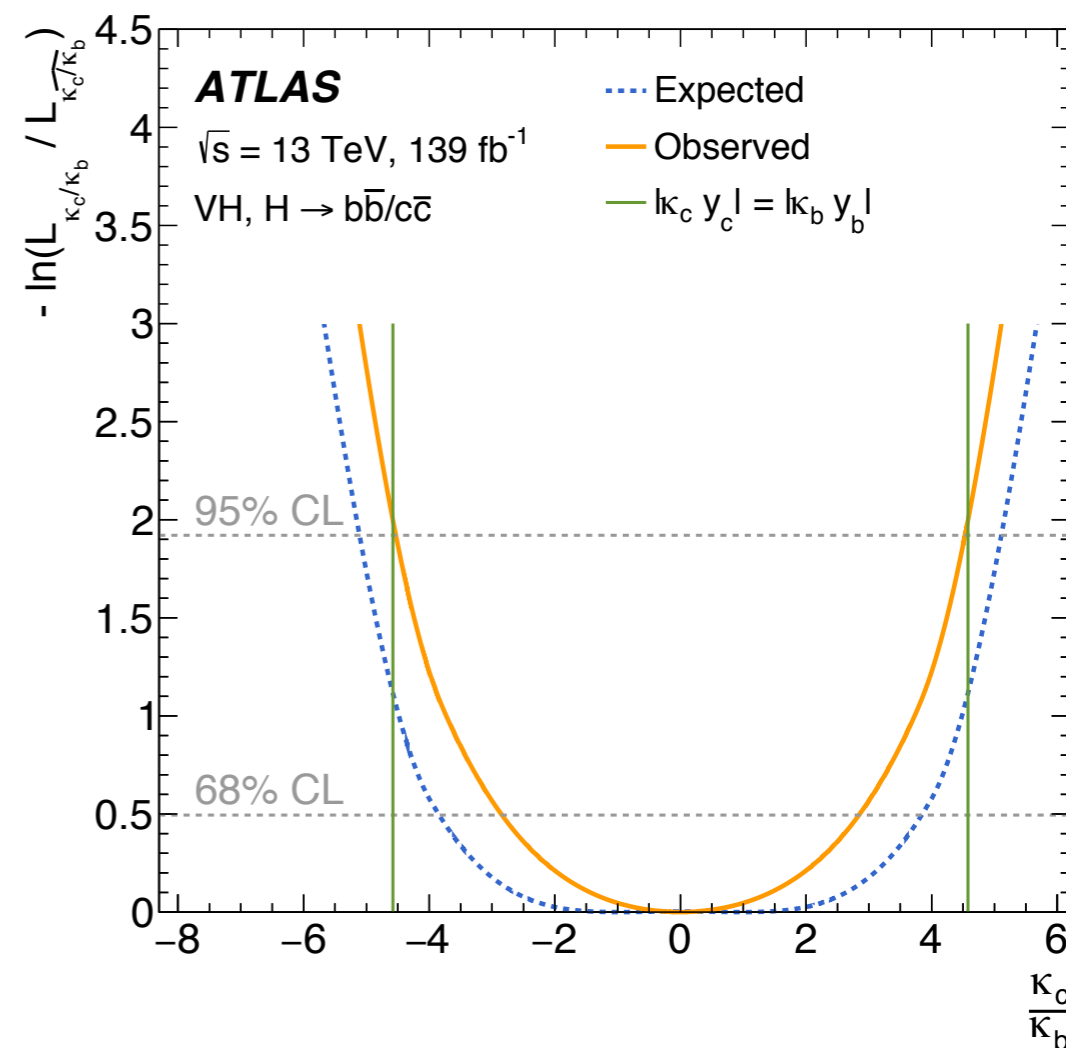
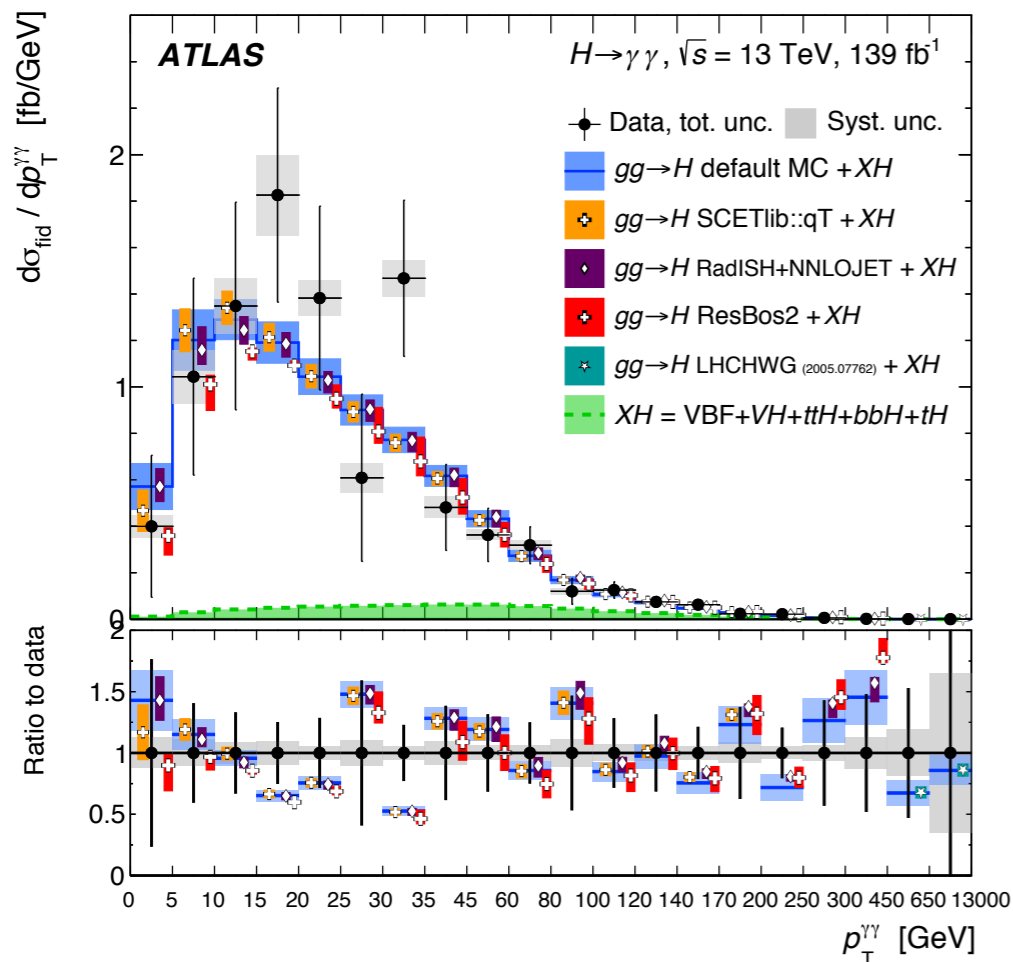
# Experiments: Recent Progress

## Measurement of $gg \rightarrow H(\rightarrow \gamma\gamma)$

$$\sigma_{\text{fid}}^{\text{exp}} = 67 \pm 7 \text{ fb}$$

$$\sigma_{\text{fid}}^{\text{th}} = 64 \pm 4 \text{ fb}$$

Also with differential fiducial cross sections  
(to high  $p_T^{\gamma\gamma}$ !) CERN-EP-2021-227



## Direct constraint on $y_b/y_c$ from $VH(\rightarrow c\bar{c})$

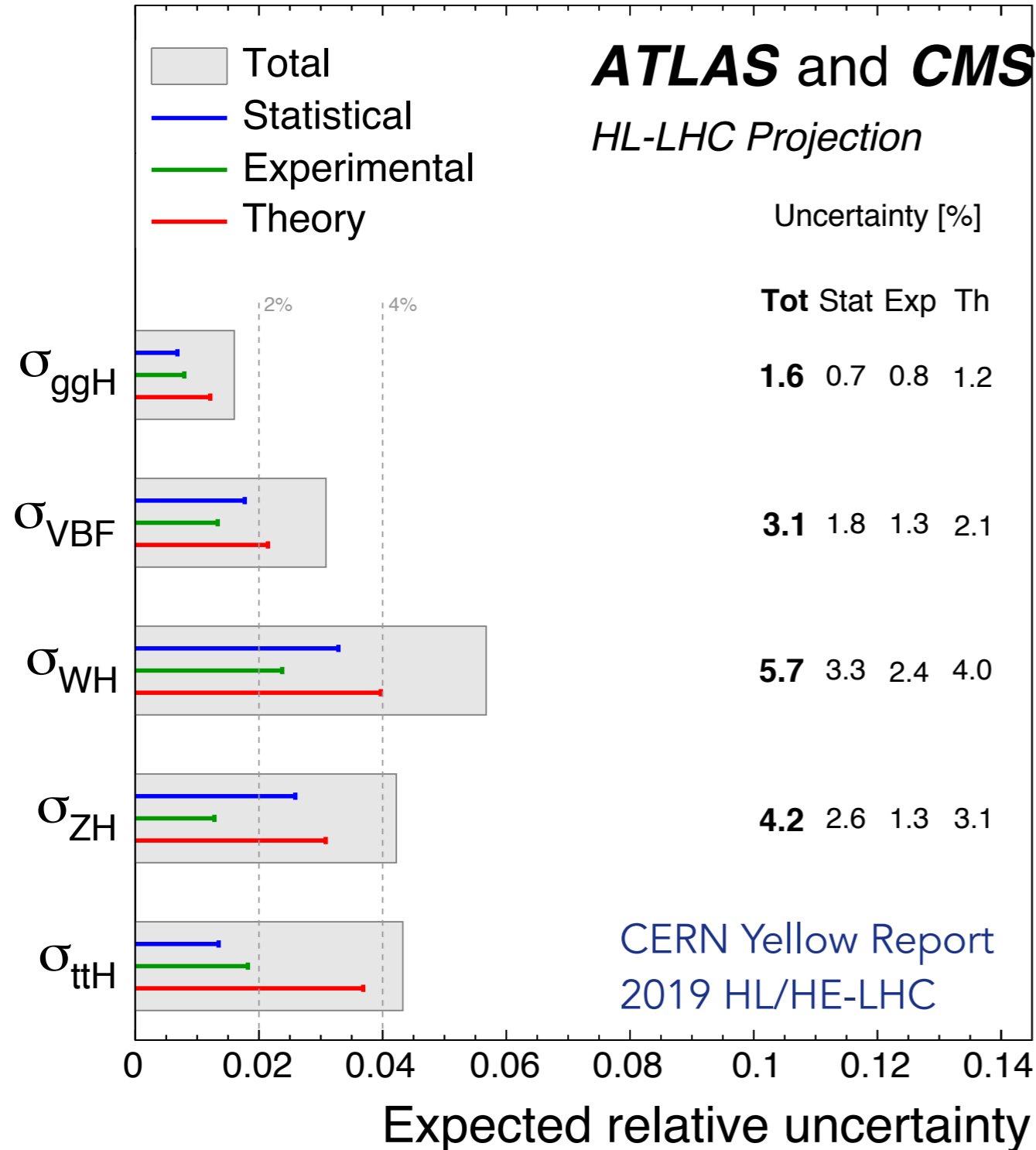
$$|\kappa_b/\kappa_c| < 4.5 < m_b/m_c \text{ @ 95\% CL}$$

Result implies that the Higgs coupling to charm quarks is smaller than the coupling to bottom quarks (as predicted by SM)

CERN-EP-2021-251

# Future Experiments: HL-LHC

$\sqrt{s} = 14 \text{ TeV}, 3000 \text{ fb}^{-1}$  per experiment



HL-LHC construction underway  
 ~10x integrated luminosity of LHC  
 (LHC  $0.3 \text{ ab}^{-1}$ , HL-LHC:  $3 \text{ ab}^{-1}$ )

**Theory uncertainty** is expected to dominate HL-LHC Higgs physics

Plot shown assumes reduction by factor 2 of today's uncertainties

# Outline

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## Motivation & Background

Higgs precision, why corrections to  $gg \rightarrow ZH$  are interesting

## Numerical calculation of Feynman integrals

Numerically evaluating amplitudes with pySecDec

Expansion by regions

## Virtual Results & Comparisons

# Motivation: Higher Order Computations

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$$d\sigma = \int dx_a dx_b f(x_a) f(x_b) d\hat{\sigma}_{ab}(x_a, x_b) F_J + \mathcal{O}((\Lambda/Q)^m)$$

Parton Distribution  
Functions (PDFs)

**Hard Scattering  
Matrix Element**

Non-perturbative  
effects ~ few %

With  $\alpha_s \sim 0.1$ , expect NLO ~ 10% correction, NNLO ~ 1% correction

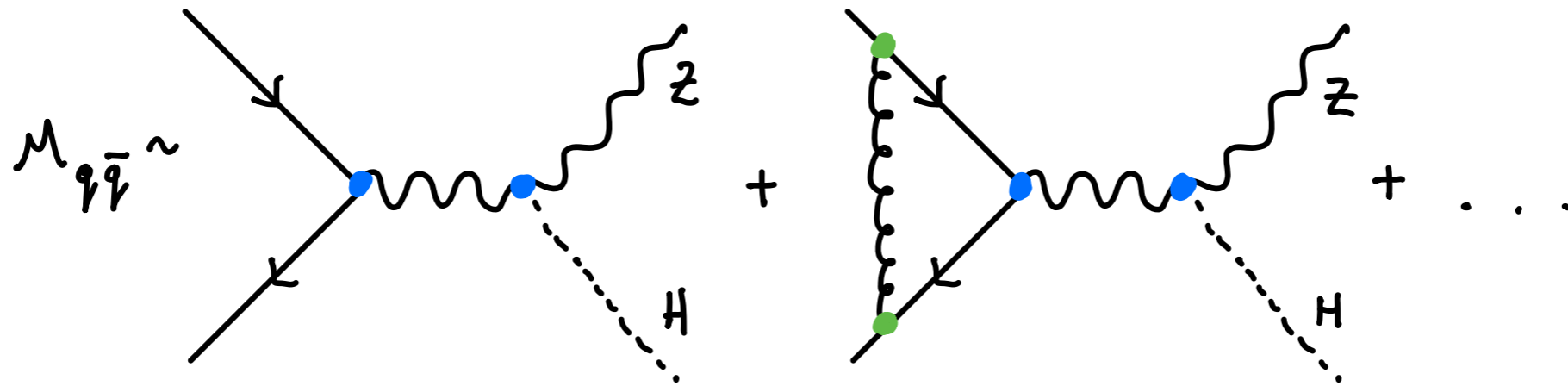
**However**, there are important exceptions:

- Higgs production (NLO ~ 100%, NNLO ~ 10%, N3LO ~ 2%)
- New partonic channels can open at higher-orders (e.g.  $gg \rightarrow ZH$ )
- Distributions can be modified substantially (even if  $\sigma_{\text{tot}}$  is stable)

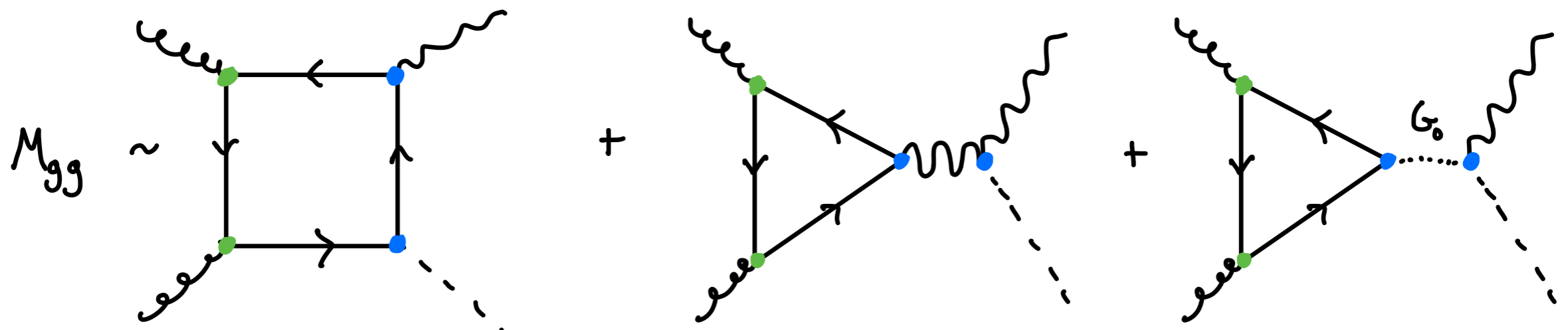
# Overview of $pp \rightarrow ZH$ (I)

Consider the matrix element for  $pp \rightarrow ZH$  with QCD corrections

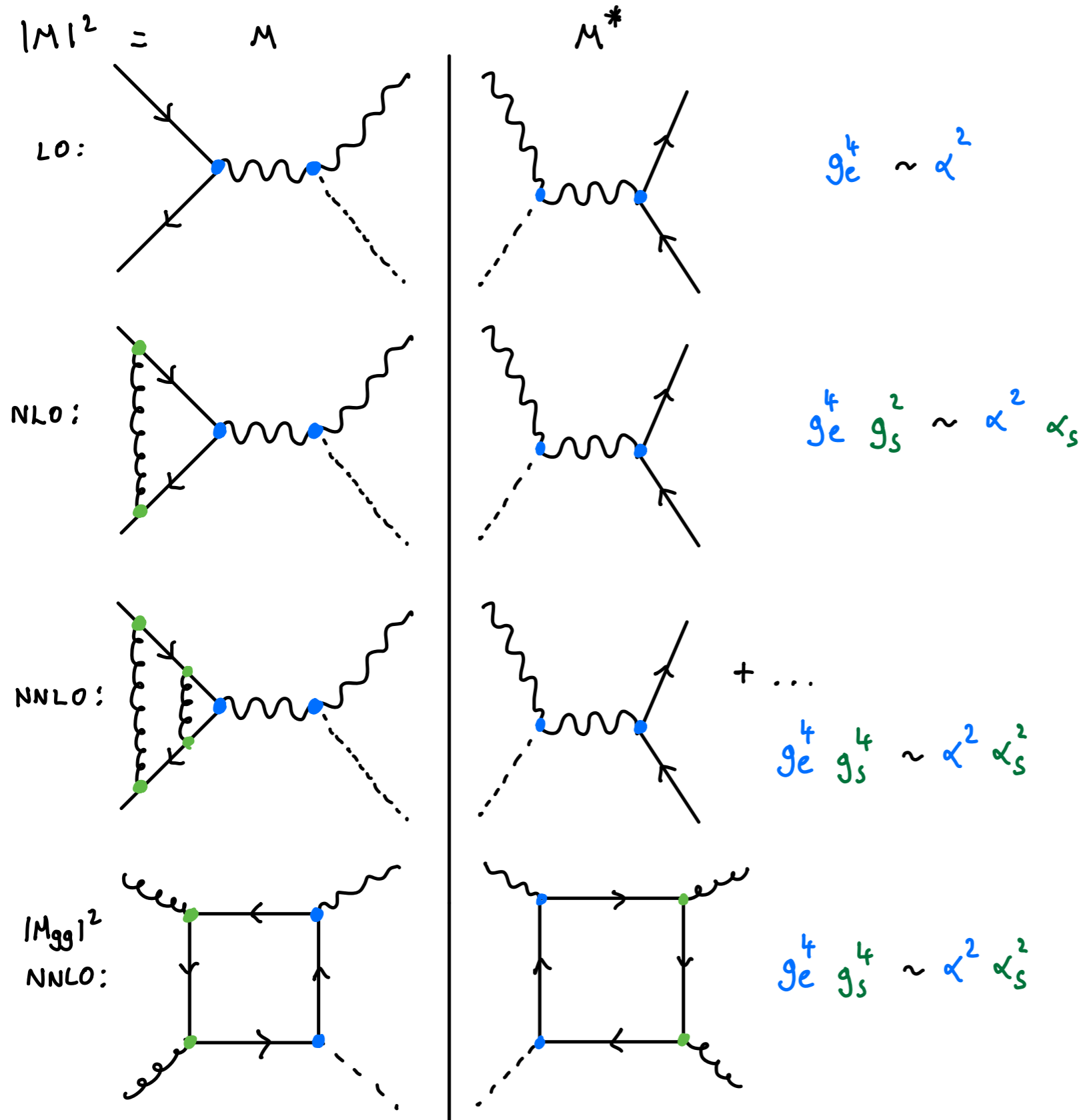
Various channels contribute:  $q\bar{q} \rightarrow ZH$  and  $gg \rightarrow ZH$



The  $gg \rightarrow ZH$  channel is **loop-induced** (i.e. LO in this channel is 1-loop)



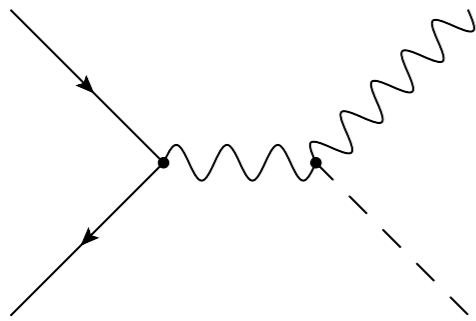
# Overview of $pp \rightarrow ZH$ (II)



The  $gg \rightarrow ZH$  channel contributes to  $pp \rightarrow ZH$  starting at NNLO in QCD

**However** due the large gluon-gluon luminosity at the LHC it contributes significantly ( $\sim 10\%$ ) to the total cross section

# Overview of $pp \rightarrow ZH$ (III)



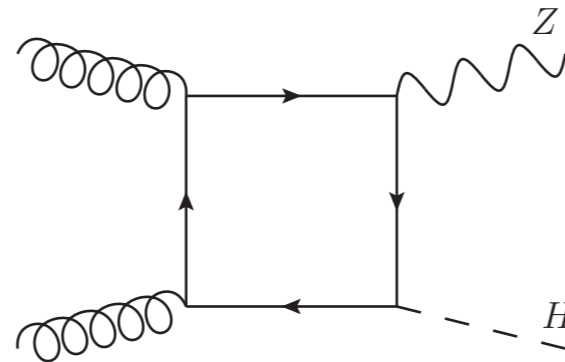
Drell-Yan piece (NNLO known)

Brein, Djouadi, Harlander 03;

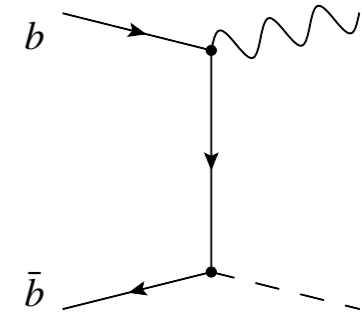
Ferrera, Grazzini, Tramontano 14;

See also: Kumara, Mandal, Ravindran 14

+  $q\bar{q}$  piece with closed top loops (1-3%)



Gluon-fusion piece



$b\bar{b}$  piece (NNLO known)

Ahmed, Ajjath, Chen, Dhani,

Mukherjee, Ravindran 19

## Available in various codes:

HAWK (NLO QCD + NLO EW)

Denner, Dittmaier, Kallweit, Mück 14

vh@nnlo (NNLO QCD + NLO EW)

Harlander, Klappert, Liebler, Simon 18;

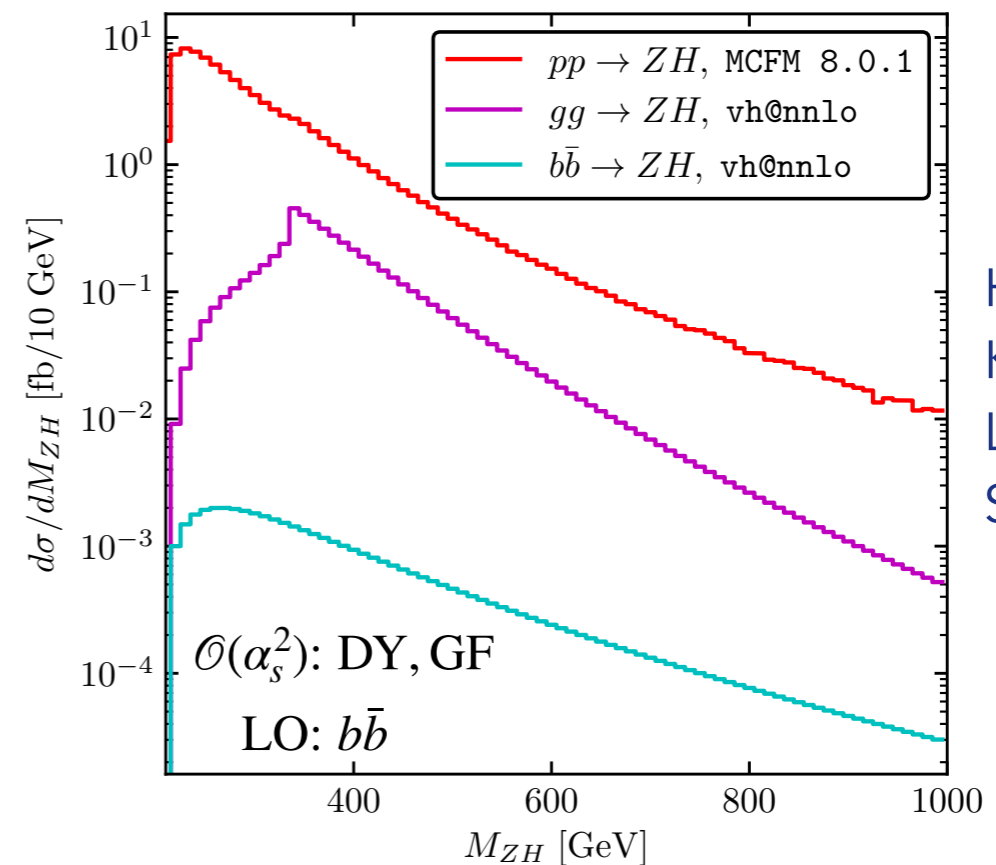
Brein, Harlander, Zirke 12

MCFM (NNLO QCD)

Campbell, Ellis, Williams 16

GENEVA (NNLL'+NNLO with PS)

Alioli, Broggio, Kallweit, Lim, Rottoli 19



Harlander,  
Klappert,  
Liebler,  
Simon 18



# Why Calculate $gg \rightarrow ZH$ ?

## The practical reason ...

~10% of total cross section

~100% scale uncertainty  
(and underestimated?)

	Signal
Cross-section (scale)	0.7% ( $qq$ ), <b>25% (<math>gg</math>)</b>
$H \rightarrow b\bar{b}$ branching fraction	1.7%
Scale variations in STXS bins	3.0%–3.9% ( $qq \rightarrow WH$ ), 6.7%–12% ( $qq \rightarrow ZH$ ), <b>37%–100% (<math>gg \rightarrow ZH</math>)</b>
PS/UE variations in STXS bins	1%–5% for $qq \rightarrow VH$ , 5%–20% for $gg \rightarrow ZH$
PDF+ $\alpha_S$ variations in STXS bins	1.8%–2.2% ( $qq \rightarrow WH$ ), 1.4%–1.7% ( $qq \rightarrow ZH$ ), 2.9%–3.3% ( $gg \rightarrow ZH$ )
$m_{bb}$ from scale variations	M+S ( $qq \rightarrow VH$ , $gg \rightarrow ZH$ )
$m_{bb}$ from PS/UE variations	M+S
$m_{bb}$ from PDF+ $\alpha_S$ variations	M+S
$p_T^V$ from NLO EW correction	M+S

ATLAS 2007.02873

### ATLAS and CMS use $ggZH@LO(QCD)$ from POWHEG

[inclusive calculation: NLO + NLL (QCD)]

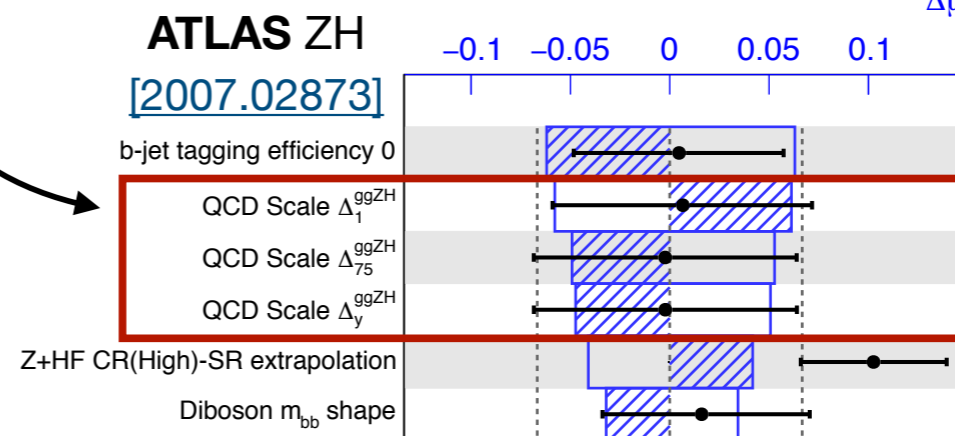
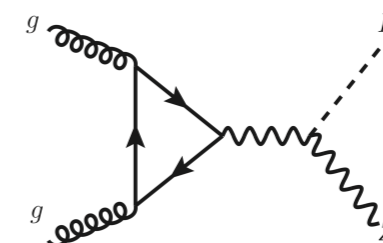
→ Large scale uncertainties

**ggZH accounts only for ~10%  
of inclusive ZH cross section**

*Uncertainties still very important!*

No full NLO calculation available  
for the foreseeable future (?)

**How to improve?**

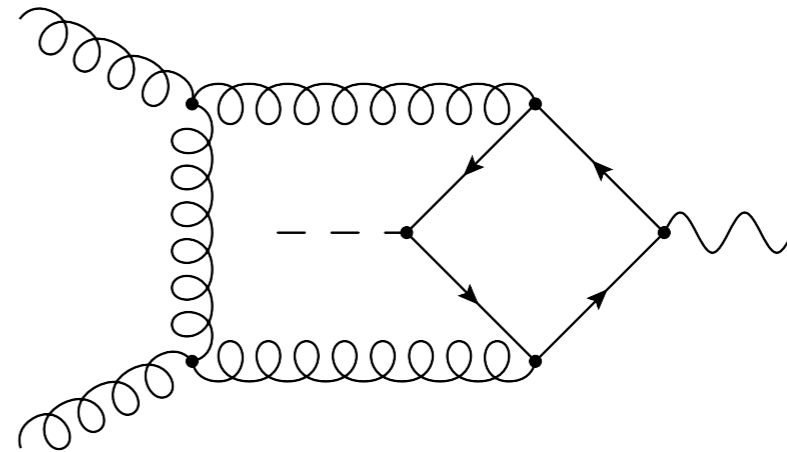
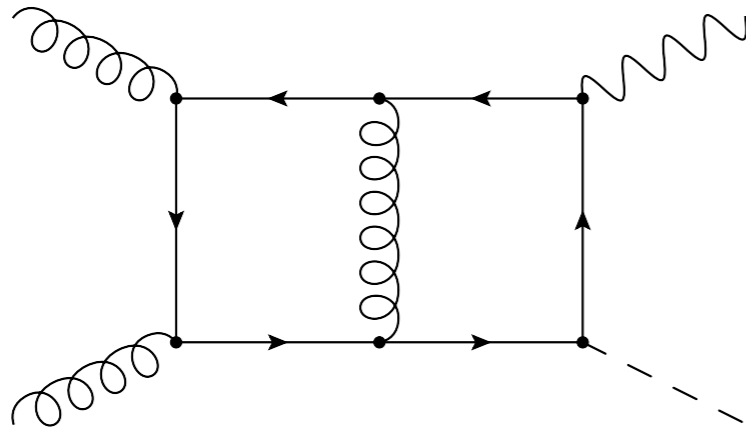


Philipp Windischhofer / ATLAS (LHCXSWG Meeting 9/11/2020)

# Why Calculate $gg \rightarrow ZH$ ? (II)

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And another reason...



**Provides new and interesting challenges:**

Amplitude depends on large number of scales  $s, t, m_Z^2, m_H^2, m_T^2$

Feynman Integrals appearing are non-trivial (internal masses, elliptic...)

**Can test our techniques to breaking point then develop new approaches!**

Can we find a basis of integrals with simple coefficients?

How can we obtain a reduction to a finite basis (many dots/numerators)?

Can we improve numerical performance near thresholds? ...

# ZH in Gluon Fusion

Full leading order (loop induced)

Dicus, Kao 88; Kniehl 90

NLO in the limit of  $m_t \rightarrow \infty$  ( $K \approx 2$ )

(asymptotic expansion)

Altenkamp, Dittmaier, Harlander, H. Rzehak, Zirke 12

## Virtual Corrections:

Expansion around large top quark mass

( $1/m_t^8$ ) + Padé approx

Hasselhuhn, Luthe, Steinhauser 17

Expansion around small top quark mass

( $1/m_t^{10}$  &  $m_t^{32}$ ) + Padé approx

Davies, Mishima, Steinhauser 20

Expansion around small  $p_T$  up to  $p_T^4$

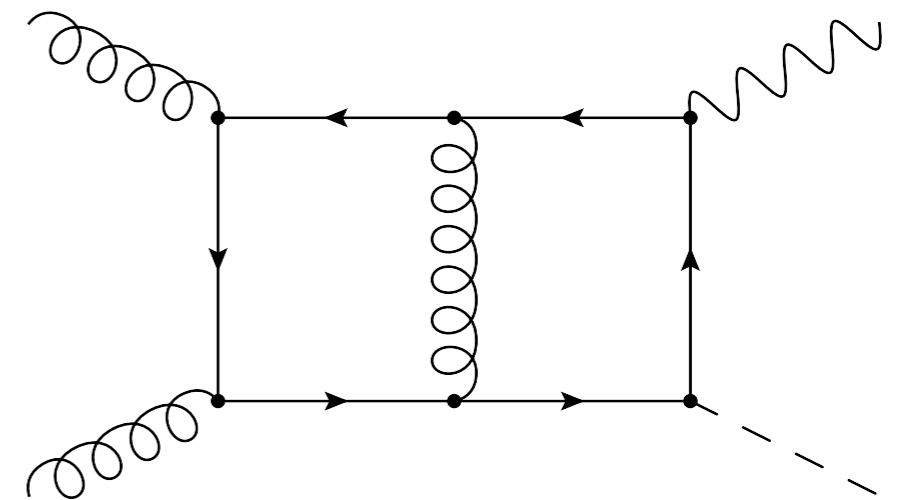
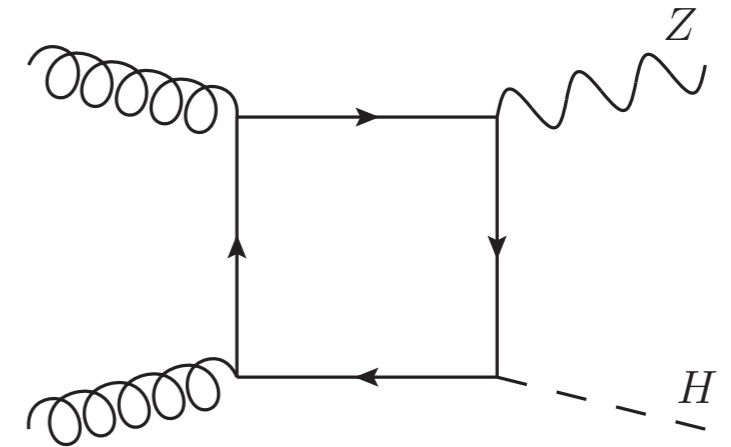
Alasfar, Degrandi, Giardino, Gröber, Vitti 21

Full numerical result

Chen, Heinrich, SPJ, Kerner, Klappert, Schlenk 20

**NLO result:** Expansion around small  $m_z, m_h$

Wang, Xu, Xu, Yang 21 (2107.08206)

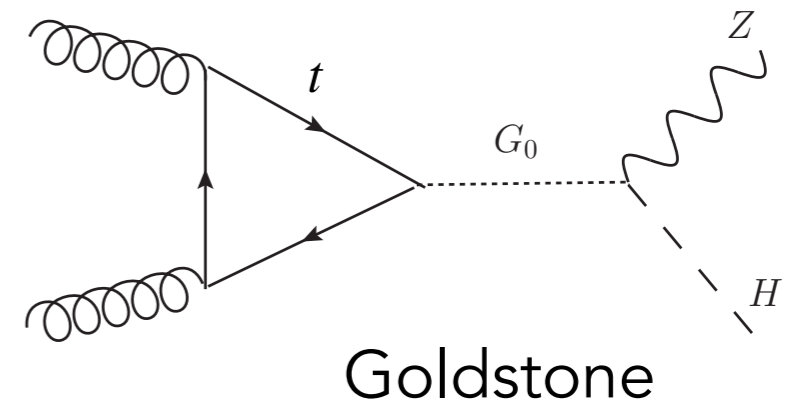
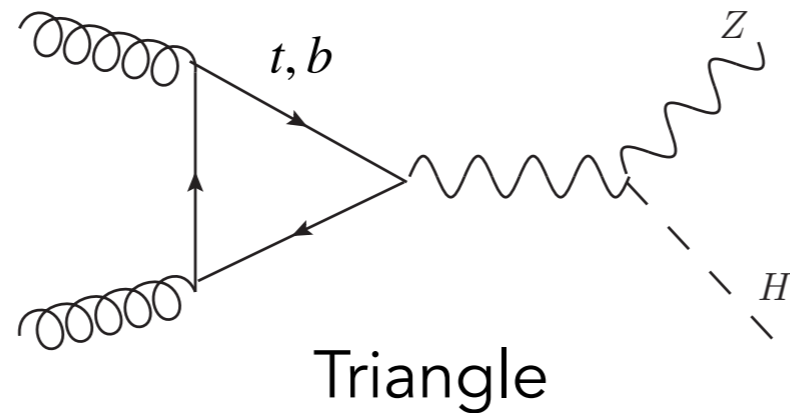
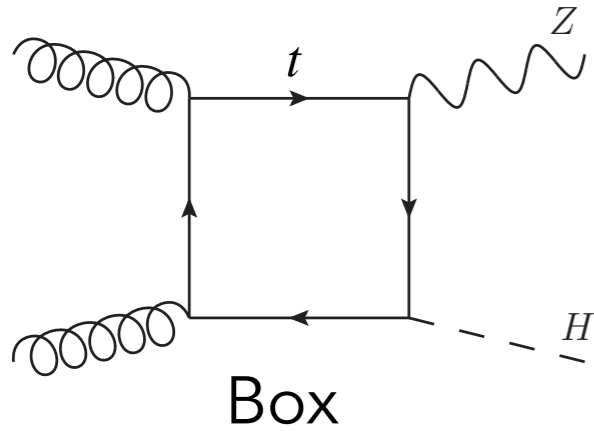


# Setup & Amplitudes

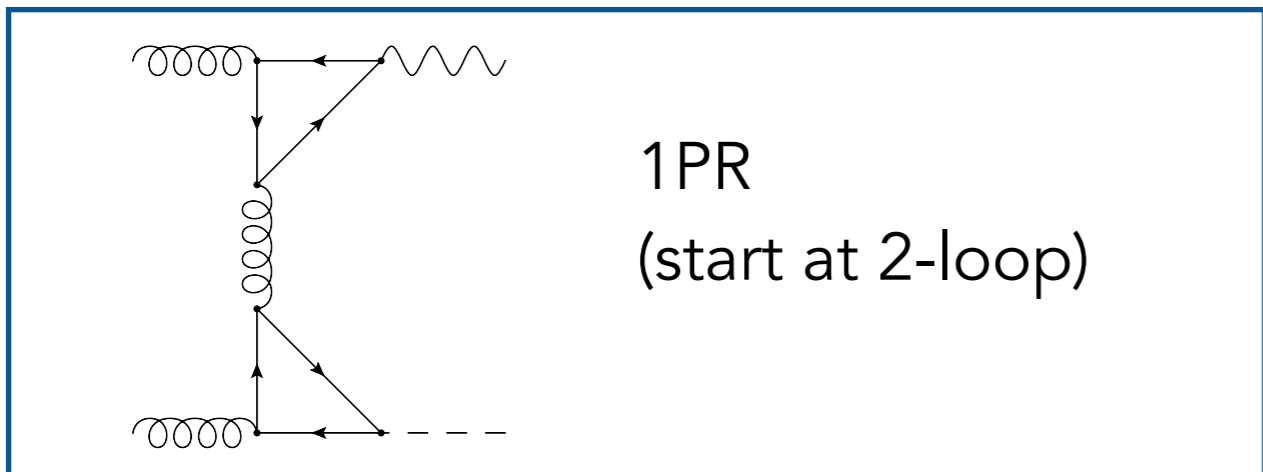
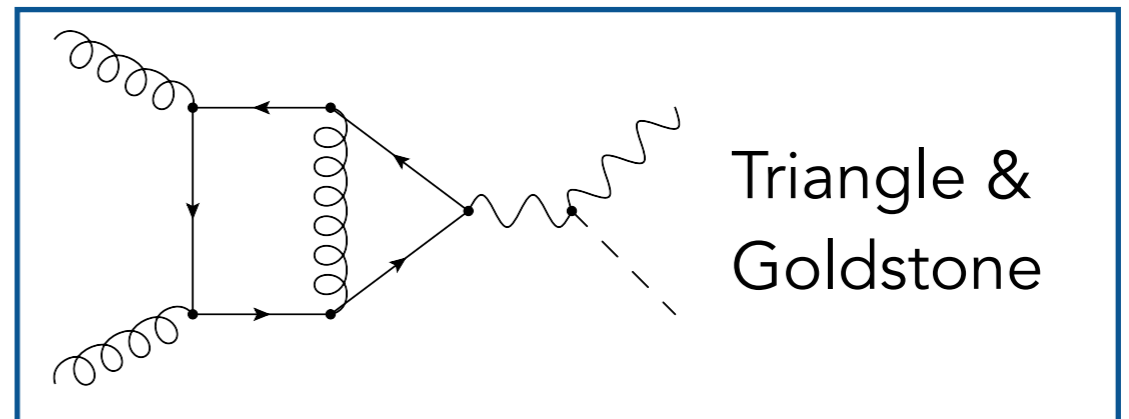
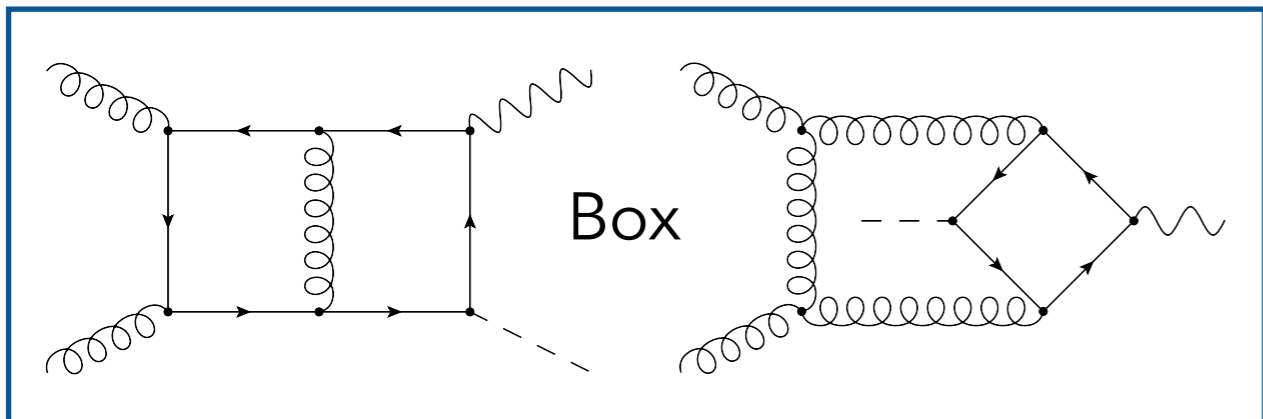
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# Diagrams: $gg \rightarrow ZH$

## Leading Order (1-loop) Diagrams



## NLO (2-loop) Virtual Diagrams

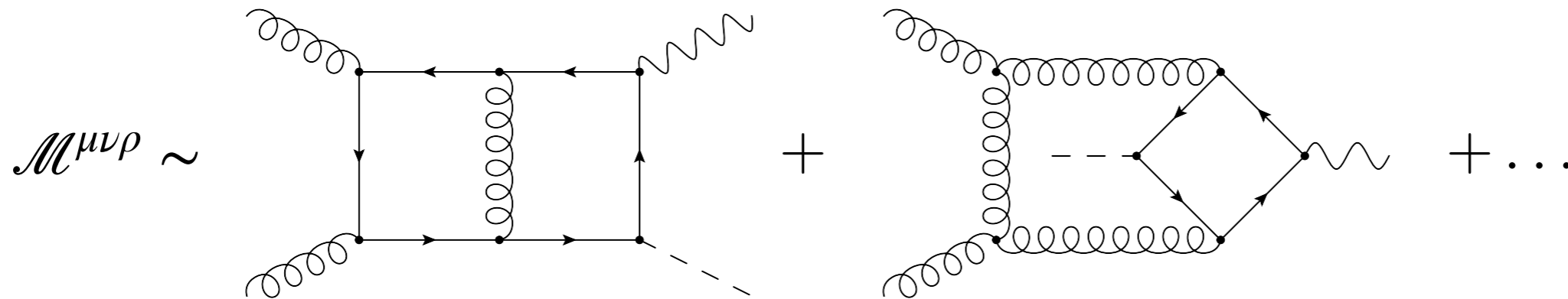


We compute in Feynman Gauge  
Keep the dependence on all EW couplings symbolic (can be varied)

Set  $m_b = 0$

# Amplitudes

Schematically:



$$\mathcal{M}^{\mu\nu\rho} = \sum_i A_i T_i^{\mu\nu\rho}, \quad A_i = \sum_k C_{i,k} I_k$$

## Rational functions

Large num. terms/ high degree  
Handled with specialist symbolic  
manipulation programs

## Feynman integrals

Analytically: Involved special functions  
(Polylogs, Elliptic...)

**In this work, we will compute them  
numerically**

# Dealing with the Integrals

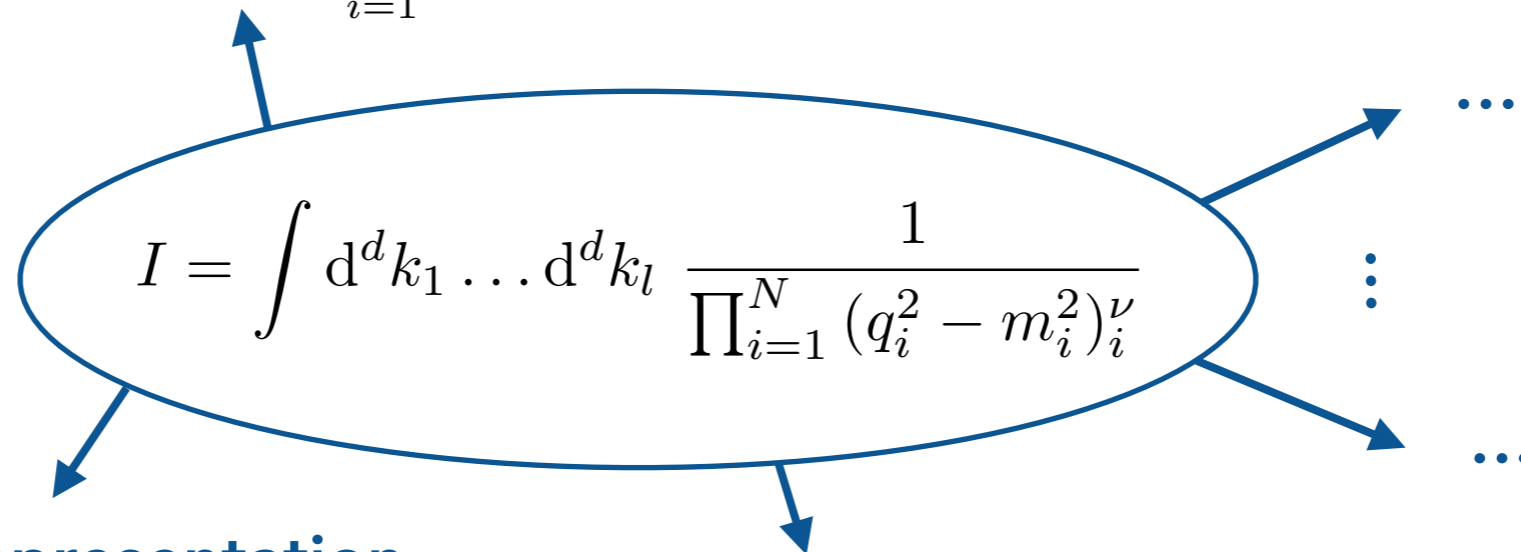
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# Feynman Integrals

Feynman integrals have many faces, each make different properties manifest...  
Switching the representation of our integrals allows us to understand/simplify/  
complete the calculation

## Feynman Parametrisation

$$I \sim \int_0^\infty \prod_{j=1}^N dx_j x_j^{\nu_1-1} \dots x_j^{\nu_N-1} \delta\left(1 - \sum_{i=1}^N x_i\right) \frac{\mathcal{U}^{N_\nu - (L+1)d/2}}{\mathcal{F}^{N_\nu - Ld/2}}$$



## Lee-Pomeransky Representation

$$I \sim \int_0^\infty \prod_{j=1}^N dx_j x_j^{\nu_1-1} \dots x_j^{\nu_N-1} G^{-D/2}$$

$$G = \mathcal{U} + \mathcal{F}$$

Lee, Pomeransky 13

## Baikov Representation

$$I \sim \int dz_1 \dots dz_N \frac{1}{\prod_{i=1}^N z_i^{\nu_i}} P^{\frac{d-L-E-1}{2}}$$

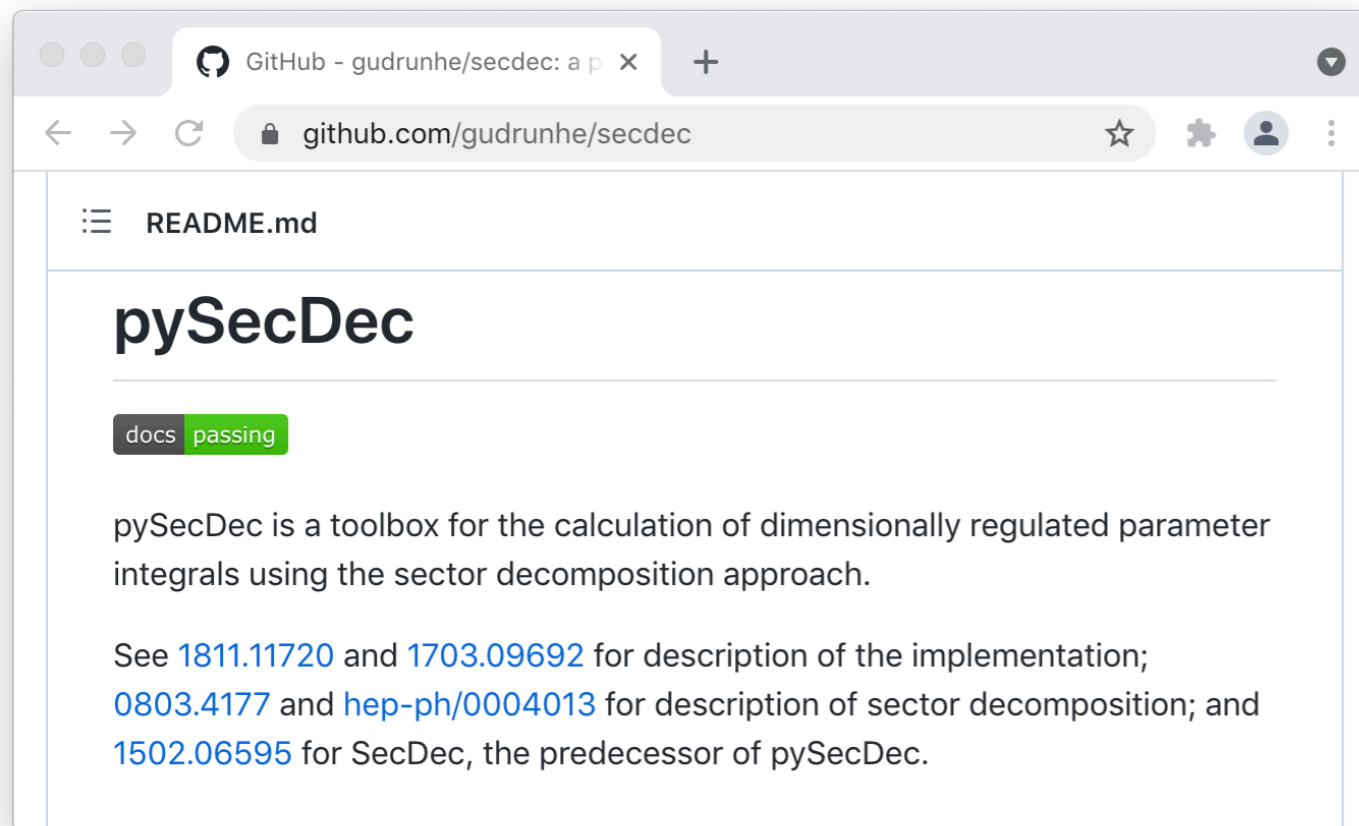
Baikov 96



# pySecDec

pySecDec: a program for numerically evaluating dimensionally regulated parameter integrals on CPU or GPU (written in python, FORM, c++, CUDA)

Vermaseren 00; Kuipers, Ueda, Vermaseren 13; Ruijl, Ueda, Vermaseren 17



Publicly available (Github)

Extensive tests (CI) and documentation

Install with:

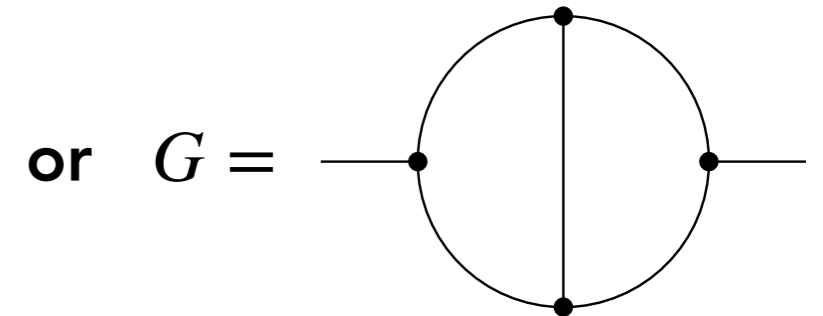
```
python3 -m pip install --user --upgrade pySecDec
```

**New:** Expansion by Regions & Amplitude Evaluation

Heinrich, Jahn, SPJ, Kerner, Langer, Magerya, Pöldaru, Schlenk, Villa 21

# Computing Integrals Numerically

**Input:**  $I = \int d^d k_1 \cdots d^d k_l \frac{1}{(k_1^2 - m^2)((k_1 - k_2)^2 - m^2)\cdots}$



Feynman Parametrise



$$\mathcal{U} = x_1 x_3 + x_1 x_4 + x_1 x_5 + \dots$$

$$\mathcal{F} = -p^2 x_1 x_2 x_3 - p^2 x_1 x_2 x_4 - \dots$$

Resolve Singularities



(Sector Decomposition)

**C++ library ready for numerical integration**

**Output:**


```
$ time python integrate_elliptic2L_euclidean.py
+ (2.47074199140731560e-01 +/- 4.36075599805171355e-16) + 0(eps)
real          0m2.576s
```

# Other Sector Decomposition Tools

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Several other codes implement sector decomposition

## Public:

- sector\_decomposition + CSectors (uses GiNaC)  
[https://particlephysics.uni-mainz.de/weinzierl/sector\\_decomposition/](https://particlephysics.uni-mainz.de/weinzierl/sector_decomposition/)  
Bogner, Weinzierl 07; Gluza, Kajda, Riemann, Yundin 10
- FIESTA (uses Mathematica, C)  **First to implement expansion by regions**  
<https://bitbucket.org/feynmanIntegrals/>  
Supports integration on GPUs  
A. Smirnov, V. Smirnov, Tentyukov 08, 09, 13, 15; Smirnov 16, 21

## (Currently) Private:

- FORM & Python Implementations  
Fujimoto, Kaneko and Ueda 08, 10
- NIFT  
Zhao (in preparation)

# New Feature 1: Amplitude Evaluation

**New release:** can evaluate entire amplitudes (used in our ZH calculation)

Let's see how this works in a simple example 1-loop 4-photon amp.

## Step 1: Define Integrals

```
import pySecDec as psd

### Integral definitions ###

I = [

    # one loop bubble (u)
    psd.loop_integral.LoopIntegralFromGraph(
        internal_lines = [[0,[1,2]],[0,[2,1]]],
        external_lines = [['p1',1],['p2',2]],
        replacement_rules = [('p1*p1', 'u'),('p2*p2', 'u'),('p1*p2', 'u')]),

    # one loop bubble (t)
    psd.loop_integral.LoopIntegralFromGraph(
        internal_lines = [[0,[1,2]],[0,[2,1]]],
        external_lines = [['p1',1],['p2',2]],
        replacement_rules = [('p1*p1', 't'),('p2*p2', 't'),('p1*p2', 't')]),

    # one loop box (in 6 dimensions)
    psd.loop_integral.LoopIntegralFromGraph(
        internal_lines = [['0',1],[1,2],[2,3],[3,4],[4,1]],
        external_lines = [['p1',1],['p2',2],['p3',3],['p4',4]],
        replacement_rules = [
            ('p1*p1', 0), ('p2*p2', 0),
            ('p3*p3', 0), ('p4*p4', 0),
            ('p3*p2', 'u/2'), ('p1*p2', 't/2'),
            ('p1*p4', 'u/2'), ('p1*p3', '-u/2-t/2'),
            ('p2*p4', '-u/2-t/2'), ('p3*p4', 't/2')
        ],
        dimensionality= '6-2*eps'
    ),

    # one loop box (in 8 dimensions)
    # ...

]
```

**Usual pySecDec Syntax**

## Step 2: Define Coefficients

```
from pySecDec import Coefficient

### Coefficients definitions ###

coeff = [
    # M+--+
    [
        # bubble (u) coefficient
        Coefficient(['-8*(t-u)'], ['-u-t'], ['t', 'u']),
        # bubble (t) coefficient
        Coefficient(['-8*(u-t)'], ['-u-t'], ['t', 'u']),
        # box6 coefficient
        Coefficient(['-8*(t**2+u**2)'], ['-u-t'], ['t', 'u']),
        # box8 coefficient
        Coefficient(['-8*3*(2*eps)'], ['1'], ['t', 'u'])
    ]
]
```

**Numerator**      **Denominator**

**Variables**

Supports:

Multiple regulators & variables

Coeffs with poles in regulators

Multiple amplitudes at once

# Amplitude Evaluation (II)

## Step 3: Generate

```
from pySecDec.loop_integral import LoopPackage
from pySecDec.code_writer import sum_package

# import integrals and coefficients
import integrals
import coefficients

# 4-photon amplitude M++-

if __name__ == '__main__':

    # define input to loop_package
    package_generators = []
    names = ['bubble_u', 'bubble_t', 'box_6', 'box_8']
    for name, integral in zip(names, integrals.I):
        package_generators.append(
            LoopPackage(
                name = name,
                loop_integral = integral,
                requested_orders = [0]
            )
        )

    # generate code sum of (int * coeff)
    sum_package(
        'yyyy1L',
        package_generators,
        regulators = ['eps'],
        requested_orders = [0],
        real_parameters = ['t', 'u'],
        coefficients = coefficients.coeff,
        complex_parameters = []
    )
```

← List of requested integrals

← Pass integrals & coefficients

## Step 4: Integrate

```
import math
from pySecDec.integral_interface import IntegralLibrary

if __name__ == "__main__":

    # load c++ library
    amp = IntegralLibrary('yyyy1L/yyyy1L_pylink.so')

    # choose Qmc integrator
    amp.use_Qmc()

    # integrate
    _, _, result = amp([-1.3,-0.8]) # t, u

    # print result
    print('Numerical Result:', result)
```

← Uses all GPUs/ CPUs on machine

Usual pySecDec Syntax

## Step 5: Generate, Compile, Run, ..., Profit!

```
$ python3 generate_yyyy1L.py
$ export CXX=nvcc
$ export SECDEC_WITH_CUDA_FLAGS="-gencode arch=compute_70,code=sm_70"
$ make -C yyyy1L -j 8
$ time python3 integrate_yyyy1L.py
> Numerical Result:
+ ((4.44089209850062616e-16,0.000000000000000000e+00)
+/- (2.30780196667706177e-16,0.000000000000000000e+00))*eps^-1

+ ((-2.84315958344628044e+01,-1.77910044838014154e-10)
+/- (4.25673251664533604e-09,2.41058630701162800e-09))

+ 0(eps)

real    0m0.764s
user    0m2.884s
sys     0m0.188s
```

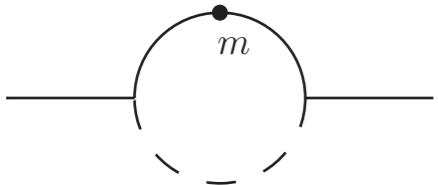
← Timings on laptop CPU

# New Feature 2: Expansion by Regions

One option for dealing with numerically unstable high-energy/threshold regions is expansion by regions (**not used in our ZH calculation**)

Beneke, Smirnov 98; Rakhmetov, Pak, Jantzen, Semenova, Becher, Neubert, Broggio, Ferroglia, ...  
(See e.g. Jantzen 11 for an introduction)

**Idea:** expand integrals around some small parameter, e.g.  $m^2/p^2$



$$= \mu^{2\epsilon} \int dk \frac{1}{(k+p)^2 (k^2 - m^2)^2}$$

(hard) :  $|k^2| \gg m^2, \quad \frac{1}{(k+p)^2 (k^2 - m^2)^2} \rightarrow \frac{1}{(k+p)^2 (k^2)^2} \left( 1 + 2\frac{m^2}{k^2} + \dots \right)$

(soft) :  $|k^2|, |k \cdot p| \ll p^2, \quad \frac{1}{(k+p)^2 (k^2 - m^2)^2} \rightarrow \frac{1}{p^2 (k^2 - m^2)^2} \left( 1 - \frac{k^2 + 2p \cdot k}{p^2} + \dots \right)$

Integrate expanded integrals over full integration range, sum over all regions

Concept can be systematically applied also in Feynman parameter space

Implemented in tools such as FIESTA/ ASY/ ASY2 and now in pySecDec

Smirnov 15; Smirnov, Smirnov, Tentyukov 09;

# Feynman Integrals: Feynman Parametrisation

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Introducing Feynman parameters and integrating over momenta, we obtain

$$G = (-1)^{N_\nu} \frac{\Gamma(N_\nu - LD/2)}{\prod_{j=1}^N \Gamma(\nu_j)} \int_0^\infty \prod_{j=1}^N dx_j x_j^{\nu_j-1} \delta(1 - \sum_{i=1}^N x_i) \frac{\mathcal{U}^{N_\nu - (L+1)D/2}(\mathbf{x})}{\mathcal{F}^{N_\nu - LD/2}(\mathbf{x}, s_{ij})}$$

$L$  - # loops in Feynman integral,  $N_\nu = \sum_{i=1}^N \nu_i$  - sum of propagator powers

$\mathcal{U}, \mathcal{F}$  are **homogenous polynomials** in the Feynman parameters  $x_i$

$\mathcal{U}(\mathbf{x})$  is degree  $L$

$\mathcal{F}(\mathbf{x})$  is degree  $L + 1$

$$\mathcal{F}(\mathbf{x}, s_{ij}) = \mathcal{F}_0(\mathbf{x}, s_{ij}) + \mathcal{U}(\mathbf{x}) \sum_{i=1}^N x_i m_i^2 \quad \leftarrow \text{internal masses}$$

Both  $\mathcal{U}, \mathcal{F}_0$  are linear in each Feynman parameter

**It is straightforward to construct  $\mathcal{U}, \mathcal{F}$  from a loop integral or graphically**

# Feynman Integrals: Lee-Pomeransky Representation

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The Lee-Pomeransky representation is given by [Lee, Pomeransky 13](#)

$$G = \frac{\Gamma(D/2)}{\Gamma((L+1)D/2 - N_\nu) \prod_{j=1}^N \Gamma(\nu_j)} \int_0^\infty \prod_{j=1}^N dx_j x_j^{\nu_j-1} \left( \mathcal{G}(\mathbf{x}, s_{ij}) \right)^{-D/2}$$

$$\mathcal{G}(\mathbf{x}, s_{ij}) = \mathcal{U}(\mathbf{x}) + \mathcal{F}(\mathbf{x}, s_{ij})$$

Inserting  $1 = \int ds \delta(s - \sum x)$  and scaling  $x \rightarrow sx$  we recover Feynman's formula

In this representation, we need to consider integrals of the form

$$G = \int_0^\infty \frac{d\mathbf{x}}{\mathbf{x}} \mathbf{x}^\nu \left[ \sum_{i=1}^m c_i \mathbf{x}^{\mathbf{p}_i} \right]^{-\frac{D}{2}}, \quad \text{where} \quad \mathbf{x}^{\mathbf{a}} = \prod_{j=1}^N x_j^{a_j}$$

This is useful for two reasons:

- 1)  $\mathcal{U} + \mathcal{F}$  is typically simpler than  $\mathcal{U} \times \mathcal{F}$
- 2) Many of the arguments can apply to a more general  $\mathcal{G}$

[Semenova, A. Smirnov,  
V. Smirnov 18](#)



# Geometric Method: Set-up

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In Feynman parameter space, there is a **geometric method** for finding regions

Pak, Smirnov 10

Each region will be defined by a **region vector**  $\mathbf{v} = (v_1, \dots, v_N, 1)$ , in each region we will perform a change of variables  $x_i \rightarrow t^{v_i} x_i$  and series expand about  $t = 0$

Let us start by considering some polynomial (could be  $\mathcal{U} + \mathcal{F}$  or something more general):

$$P(\mathbf{x}, t) = \sum_{i=1}^m c_i x_1^{p_{i,1}} \cdots x_N^{p_{i,N}} t^{p_{i,N+1}}$$

$c_i$  - non-negative coefficients

$x_i$  - integration variables

$t$  - small parameter

$\mathbf{p}'_i = (p_{i,1}, \dots, p_{i,N+1}) \in \mathbb{N}^{N+1}$  - exponent vectors

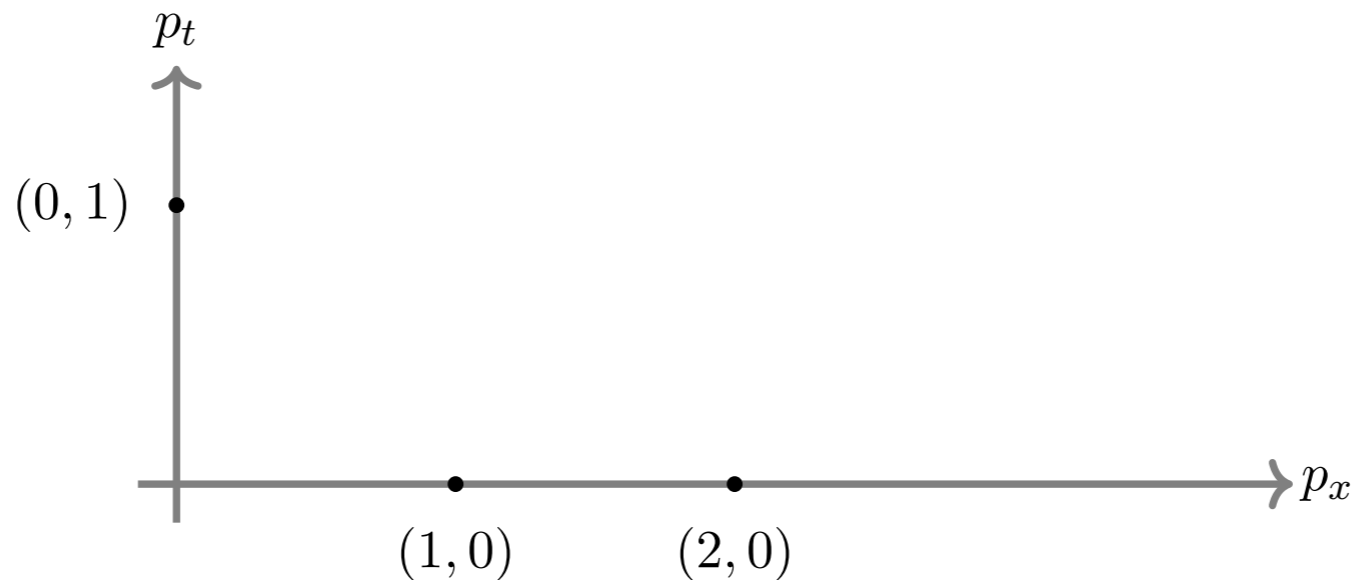
# Geometric Method: Determining the Regions

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Ignoring, for now, the coefficients  $c_i$  we can introduce a simple but useful picture for such polynomials:

- For each variable  $x_i$  or  $t$  draw an orthogonal axis
- For each monomial, draw a dot at position  $\mathbf{p}'_i$

**Example:**  $P(x, t) = t + x + x^2$  has exponent vectors  
 $\mathbf{p}'_1 = (0,1)$ ,  $\mathbf{p}'_2 = (1,0)$ ,  $\mathbf{p}'_3 = (2,0)$



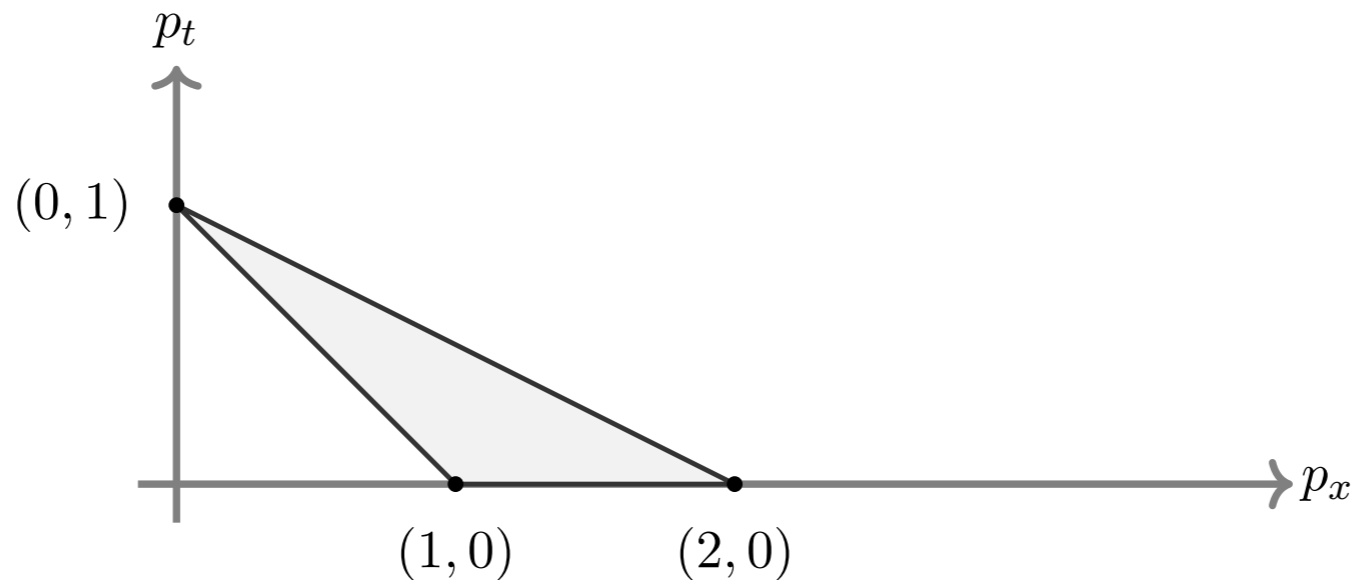
# Geometric Method: Determining the Regions (II)

We may also define a **Newton polytope** of the polynomial, this is the convex hull of the exponent vectors:

$$\Delta = \text{convHull}(\mathbf{p}'_1, \mathbf{p}'_2, \dots) = \left\{ \sum_j \alpha_j \mathbf{p}'_j \mid \alpha_j \geq 0 \wedge \sum_j \alpha_j = 1 \right\}$$

**Example:**  $P(x, t) = t + x + x^2$  has exponent vectors

$$\mathbf{p}'_1 = (0, 1), \mathbf{p}'_2 = (1, 0), \mathbf{p}'_3 = (2, 0)$$



# Geometric Method: Determining the Regions (III)

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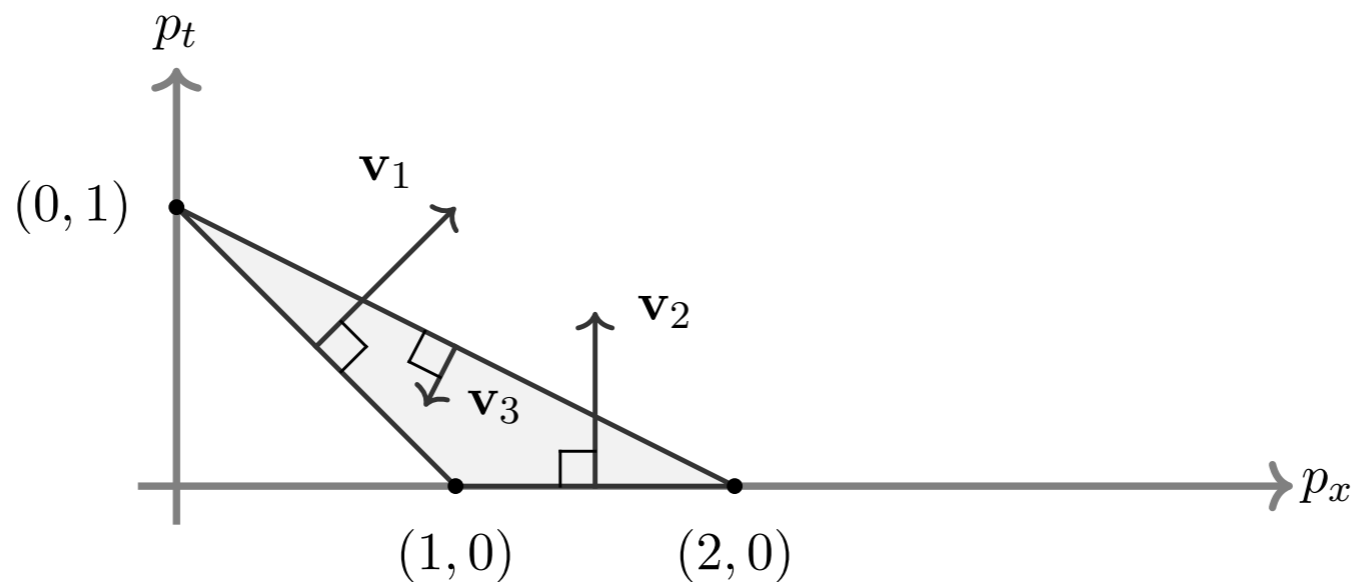
Alternatively, this polytope can also be described as the intersection of half spaces:

$$\Delta' = \bigcap_{f \in F} \left\{ \mathbf{m} \in \mathbb{R}^{N+1} \mid \langle \mathbf{m}, \mathbf{v}_f \rangle + a_f \geq 0 \right\}$$

$F$  - set of polytope facets,  $a_f \in \mathbb{Z}$

$\mathbf{v}_f$  - inward-pointing normal vectors for each facet

Several public tools exist for computing Newton polytopes/convex hulls and their representation in terms of facets exist, e.g. **Normaliz** and **Qhull**



# Geometric Method: Determining the Regions (IV)

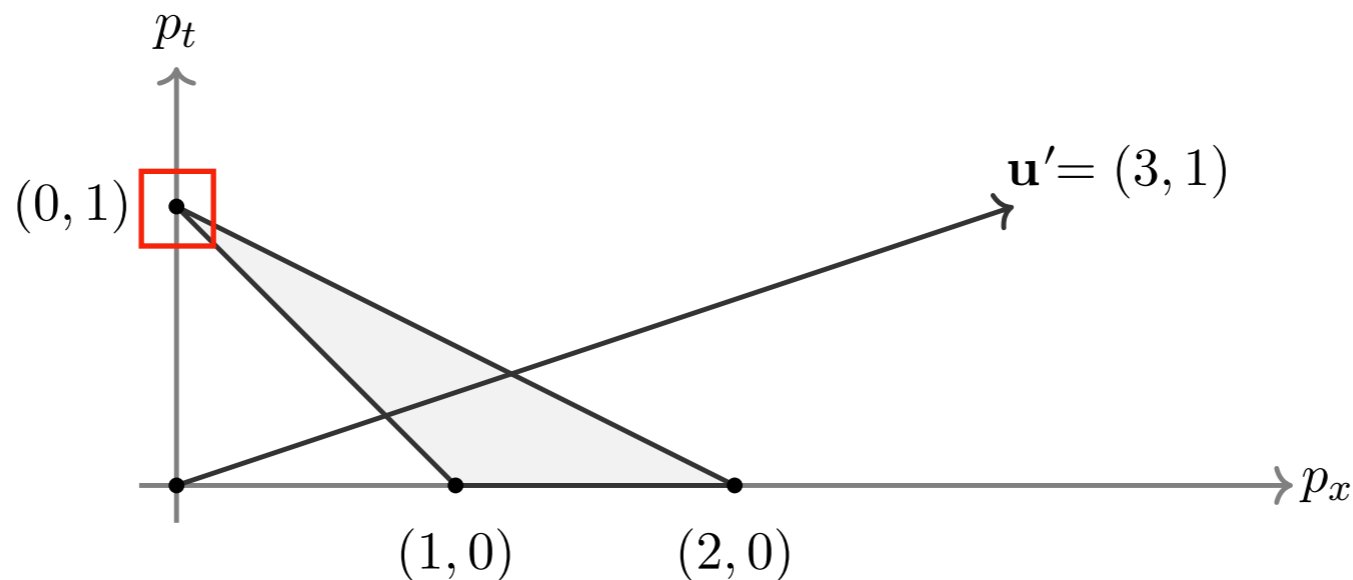
Next, let us define a vector  $\mathbf{u}$  such that  $x_i = t^{u_i}$  and a vector  $\mathbf{u}' = (\mathbf{u}, 1)$ , for each point  $\mathbf{x}$  in the integration domain, we can write:

$$P(t^{\mathbf{u}}, t) = \sum_{i=1}^m c_i t^{\langle \mathbf{p}'_i, \mathbf{u}' \rangle}$$

Since  $t \ll 1$ , the largest term in the polynomial has the smallest  $\langle \mathbf{p}'_i, \mathbf{u}' \rangle$

Note that we can have several points with the same projection on  $\mathbf{u}'$ , i.e. we can have several largest terms

**Example:**  $P(x, t) = t + x + x^2$  with  $\mathbf{u}' = (3, 1)$  gives  $P(t^{\mathbf{u}}, t) = \underline{t} + t^3 + t^6$



# Geometric Method: Determining the Regions (V)

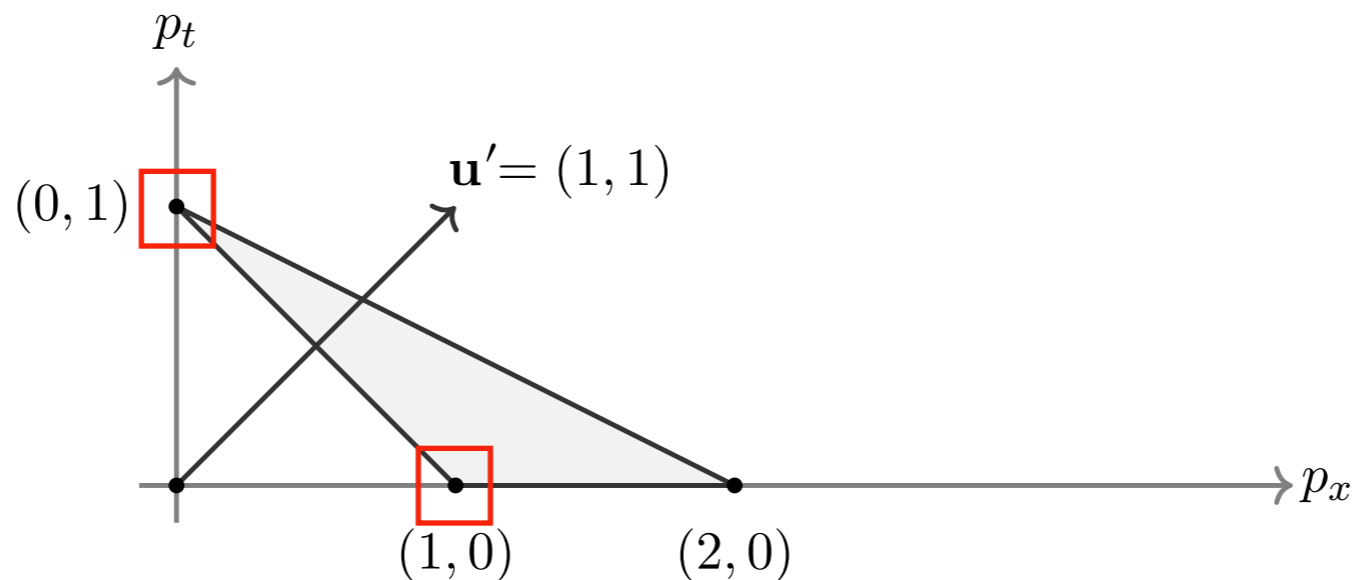
Next, let us define a vector  $\mathbf{u}$  such that  $x_i = t^{u_i}$  and a vector  $\mathbf{u}' = (\mathbf{u}, 1)$ , for each point  $\mathbf{x}$  in the integration domain, we can write:

$$P(t^{\mathbf{u}}, t) = \sum_{i=1}^m c_i t^{\langle \mathbf{p}'_i, \mathbf{u}' \rangle}$$

Since  $t \ll 1$ , the largest term in the polynomial has the smallest  $\langle \mathbf{p}'_i, \mathbf{u}' \rangle$

Note that we can have several points with the same projection on  $\mathbf{u}'$ , i.e. we can have several largest terms

**Example:**  $P(x, t) = t + x + x^2$  with  $\mathbf{u}' = (1, 1)$  gives  $P(t^{\mathbf{u}}, t) = \underline{t + t} + t^2$



# Geometric Method: Determining the Regions (VI)

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Rewrite our polynomial as:  $P(\mathbf{x}) = Q(\mathbf{x}) + R(\mathbf{x})$

With  $Q(\mathbf{x})$  defined such that it contains all of the lowest order terms in  $t$

Then, binomial expansion of

$$P(\mathbf{x})^m = Q(\mathbf{x})^m \left( 1 + \frac{R(\mathbf{x})}{Q(\mathbf{x})} \right)^m \text{ converges for } \mathbf{x} = t^{\mathbf{u}} \text{ if } R(\mathbf{x})/Q(\mathbf{x}) < 1$$

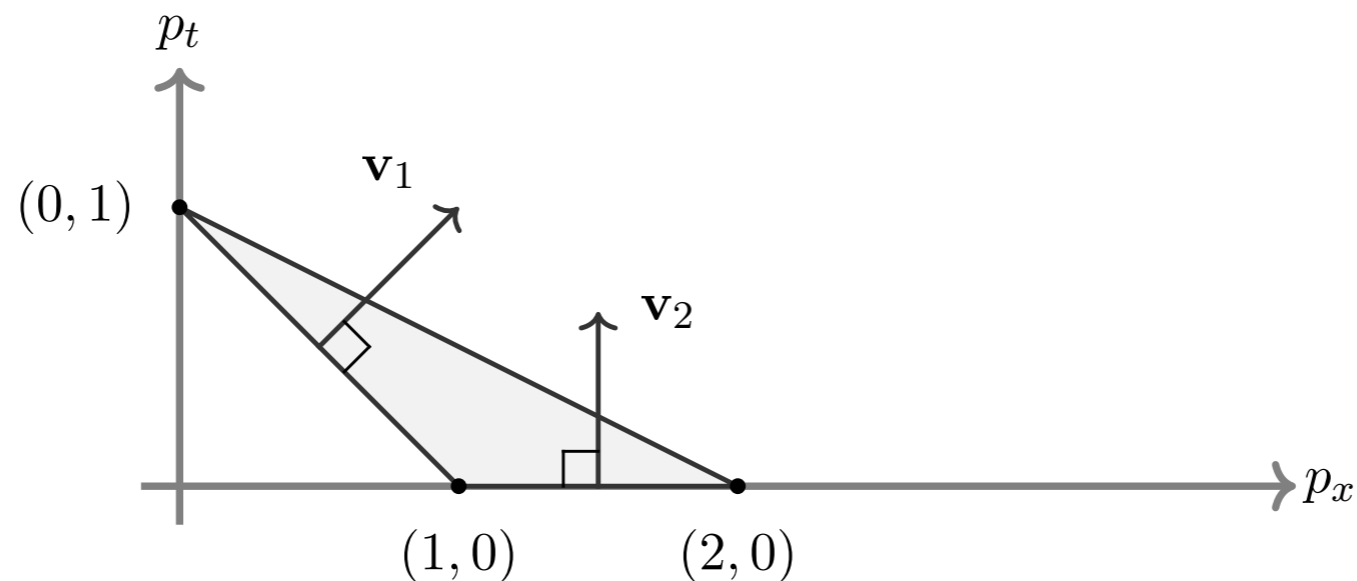
## Some observations:

- An expansion with region vector  $\mathbf{v}$  converges at a point  $\mathbf{u}'$  if the lowest order terms along the direction  $\mathbf{v}$  contain the lowest order terms along the direction  $\mathbf{u}'$
- For any direction  $\mathbf{u}'$  the vertices with the smallest  $\langle \mathbf{p}'_i, \mathbf{u}' \rangle$  must be part of some facet  $F$  of the polytope
- Since  $u_{N+1} > 0$ , the lowest order terms for any  $\mathbf{u}'$  must lie on a facet whose inwards pointing normal vector has a positive  $(N + 1)$ -th component, let us call the set of such facets  $F^+$

# Geometric Method: Determining the Regions (VII)

## How do we choose the regions?

The region vectors may be chosen as the facets whose inwards pointing normal vector has a positive  $(N + 1)$  component



Our original integral  $G$  may then be approximated as 
$$G = \sum_{f \in F^+} G^{(f)} + \dots$$

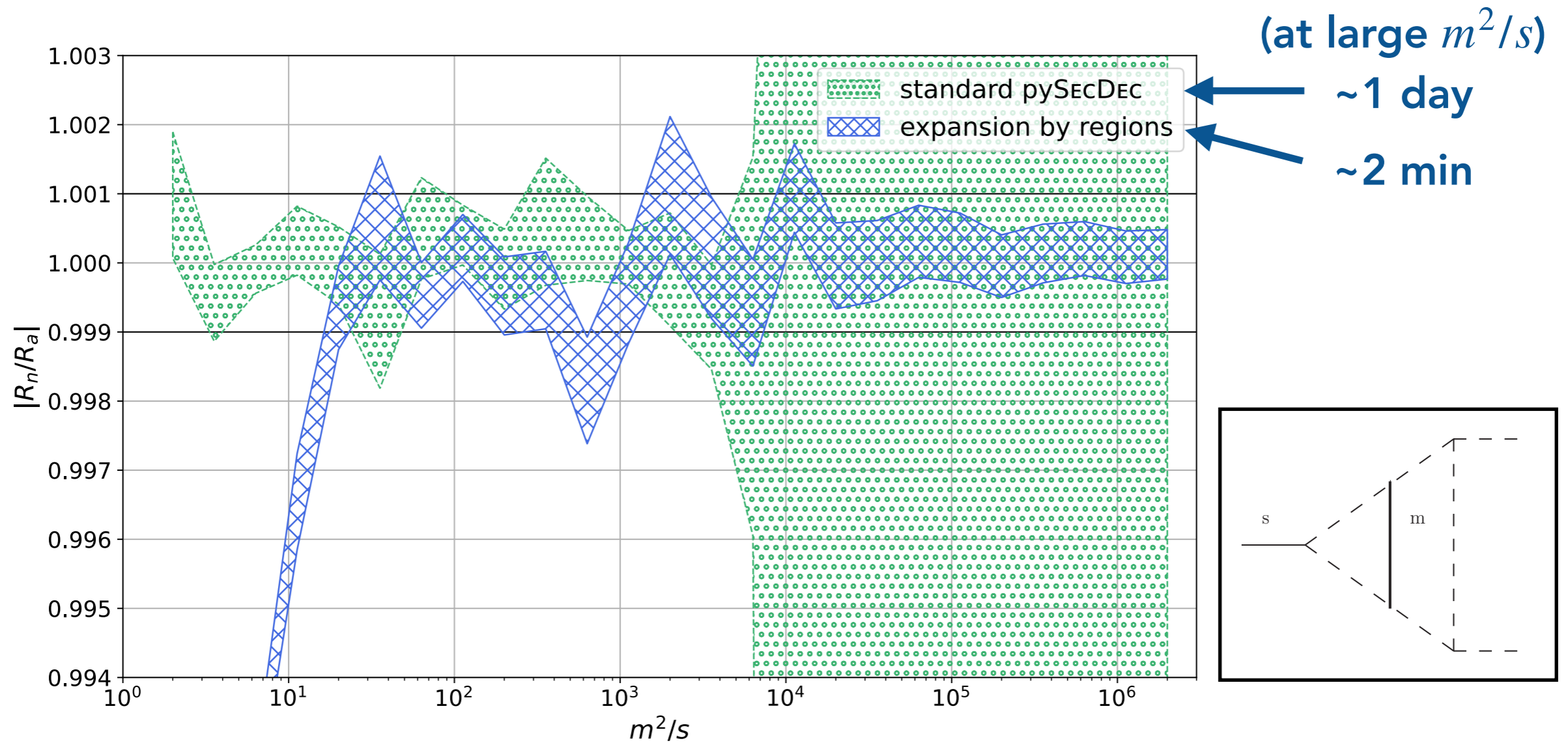
Where  $G^{(f)}$  are the series expanded integrals integrated over the whole domain

The “+...” terms are overlap contributions/ multiple expansions, for sufficiently regulated Feynman integrals (dim reg + analytic regulators) these terms are usually scaleless (=0 in dim reg) and can be neglected



# Expansion by Regions

Consider a 2-loop form factor integral, plot the ratio of the finite  $\mathcal{O}(\epsilon^0)$  piece of our numerical result  $R_n$  to the analytic result  $R_a$



Where we have a large ratio of scales ( $m^2/s$ ) the EBR result is much **faster** & **easier** to integrate

Results  $gg \rightarrow ZH$

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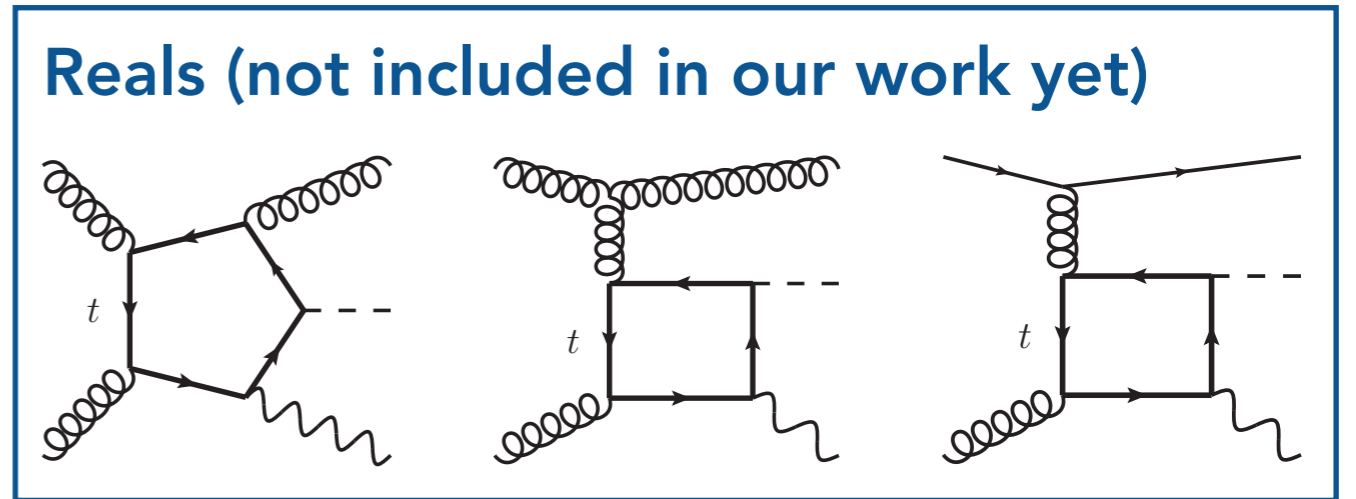
# Finite Virtual Correction

Schematically,

$$\hat{\sigma} = \hat{\sigma}^{\text{LO}} + \hat{\sigma}^{\text{NLO}}$$

$$\hat{\sigma}^{\text{LO}} = \int_n d\sigma^{\text{B}}$$

$$\hat{\sigma}^{\text{NLO}} = \int_n d\sigma^{\text{V}} + \int_{n+1} d\sigma^{\text{R}} + \int_n d\sigma^{\text{C}}$$



Virtual part ( $d\sigma^{\text{V}}$ ) and real part ( $d\sigma^{\text{R}}$ ) not separately finite for  $\epsilon \rightarrow 0$

However, we can define a finite virtual contribution as follows:

- 1) UV renormalize:  $\alpha_s$  in  $\overline{\text{MS}}$  & top quark mass in OS scheme
- 2) IR structure well known at NLO, subtract divergences

$$\mathcal{A}_i^{(0),\text{fin}} = \mathcal{A}_i^{(0),\text{UV}},$$

$$\mathcal{A}_i^{(1),\text{fin}} = \mathcal{A}_i^{(1),\text{UV}} - I_1 \mathcal{A}_i^{(0),\text{UV}},$$

$$I_1 = I_1^{\text{soft}} + I_1^{\text{coll}},$$

$$I_1^{\text{soft}} = -\frac{e^{\epsilon\gamma_E}}{\Gamma(1-\epsilon)} \left(\frac{\mu_R^2}{s}\right)^\epsilon \left(\frac{1}{\epsilon^2} + \frac{i\pi}{\epsilon}\right) 2C_A,$$

$$I_1^{\text{coll}} = -\frac{\beta_0}{\epsilon} \left(\frac{\mu_R^2}{s}\right)^\epsilon.$$

# A Few Conventions

We present results for the Born and Born-Virtual interference helicity amplitudes

**Expand the helicity amplitudes in  $\alpha_s$**

$$\mathcal{A}_{\lambda_1\lambda_2\lambda_3}^{\text{fin}} = \left(\frac{\alpha_s}{4\pi}\right) \mathcal{A}_{\lambda_1\lambda_2\lambda_3}^{(0),\text{fin}} + \left(\frac{\alpha_s}{4\pi}\right)^2 \mathcal{A}_{\lambda_1\lambda_2\lambda_3}^{(1),\text{fin}} + \dots$$

**Compute the square/interference**

$$\mathcal{B} = \frac{1}{4} \sum_{\lambda_1\lambda_2\lambda_3} |\mathcal{A}_{\lambda_1\lambda_2\lambda_3}^{(0),\text{fin}}|^2,$$

$$\mathcal{V} = \frac{1}{4} \sum_{\lambda_1\lambda_2\lambda_3} 2 \operatorname{Re} \left( \mathcal{A}_{\lambda_1\lambda_2\lambda_3}^{*(0),\text{fin}} \mathcal{A}_{\lambda_1\lambda_2\lambda_3}^{(1),\text{fin}} \right)$$

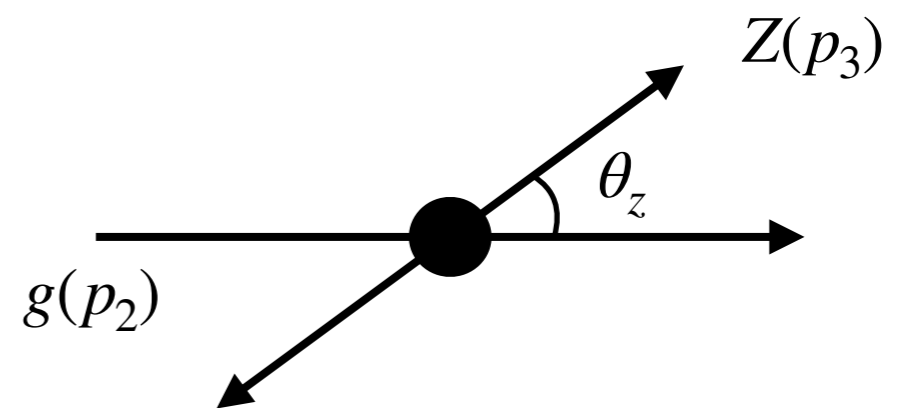
Renormalization scale set to  $\mu_R^2 = s$   
Electroweak coupling  $e^2 = 4\pi\alpha = 1$   
(can easily vary couplings/scales)

$2 \rightarrow 2$  amplitude depends on two kinematic variables (after fixing masses)

**Choose:**

$$s = (p_1 + p_2)^2$$

$\theta_z$  - angle in c.o.m frame between  $p_2$ -axis and  $p_3$



# Evaluation of the Amplitude

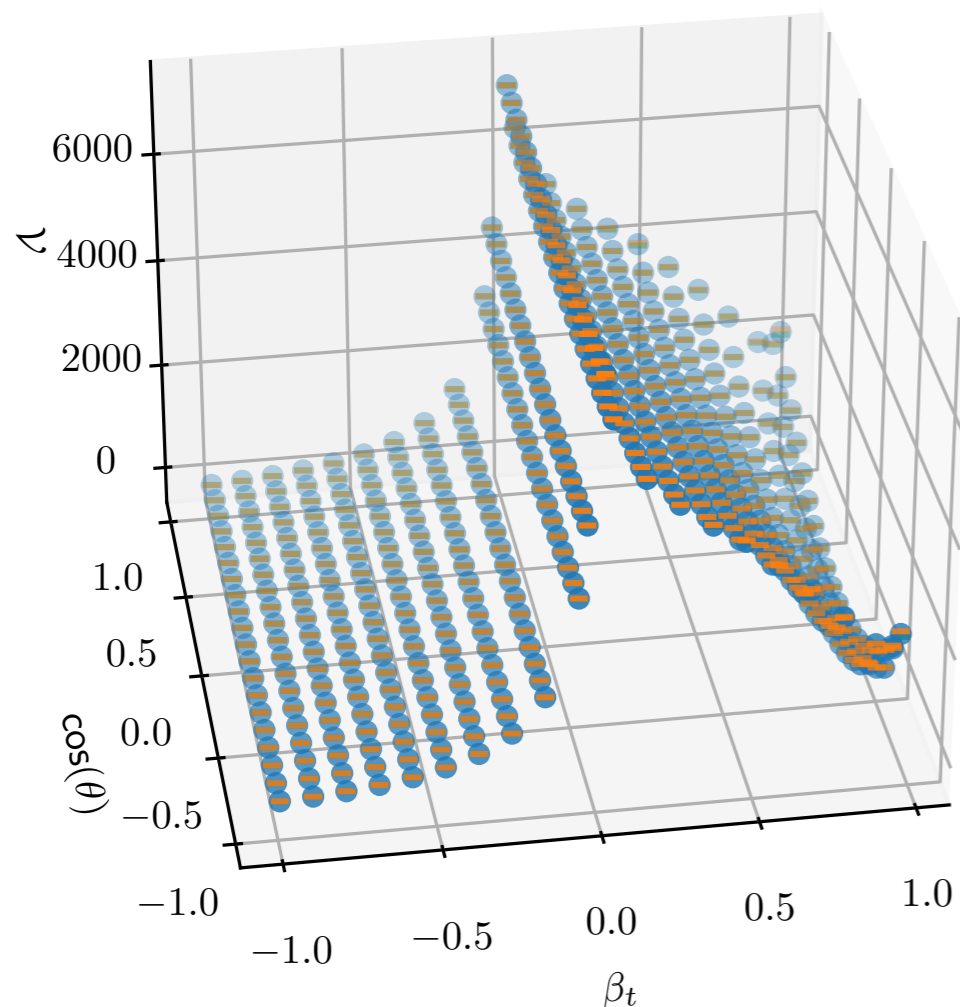
Again,  $2 \rightarrow 2$  amplitude depends on two kinematic variables (after fixing masses)

$$\beta_t = \frac{s - 4m_t^2}{s + 4m_t^2 - (2m_z + m_h)^2}, \quad \theta_z \text{ - angle in c.o.m frame}$$

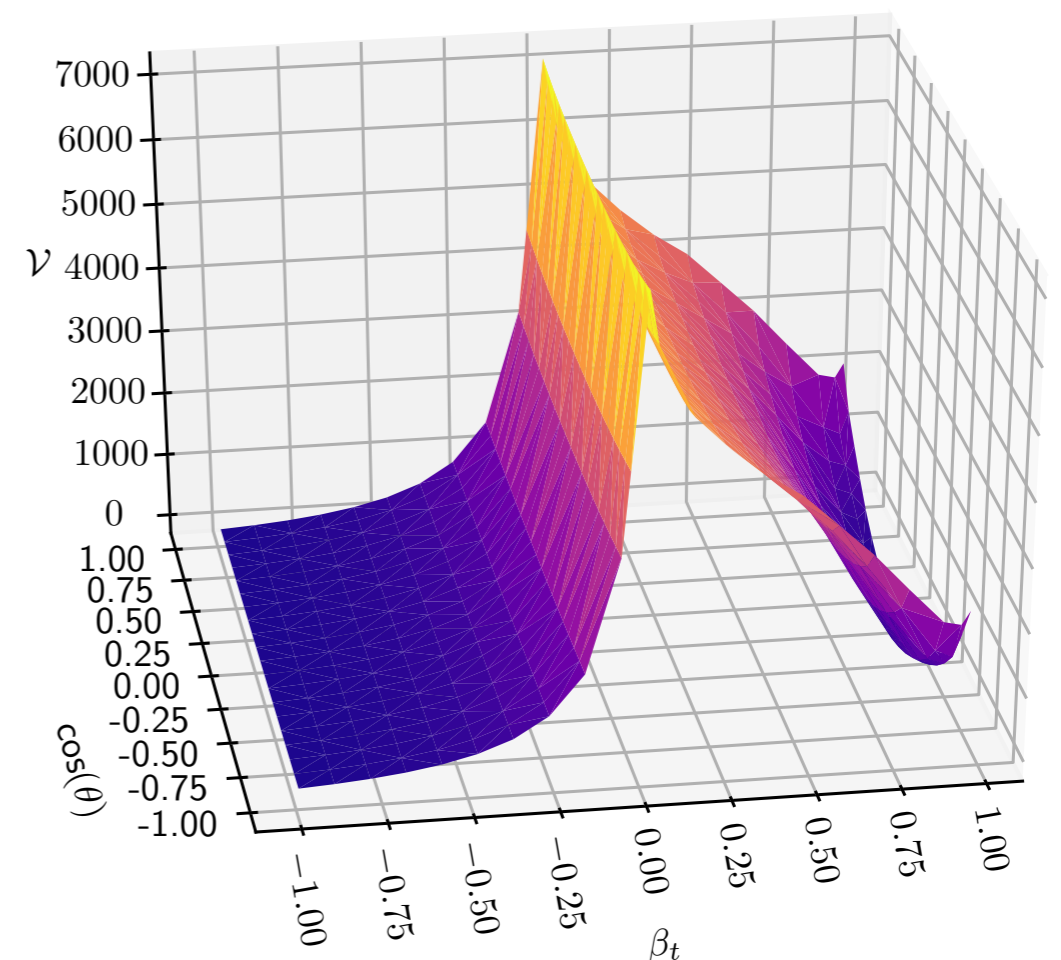
between  $p_2$ -axis and Z-boson ( $p_3$ )

Sample grid of  $20 \times 20$  points + 80 extra top threshold/high-energy points in range:

$$-0.99 < \beta_t < 0.99 \text{ and } -0.99 < \cos(\theta_z) < 0.99$$

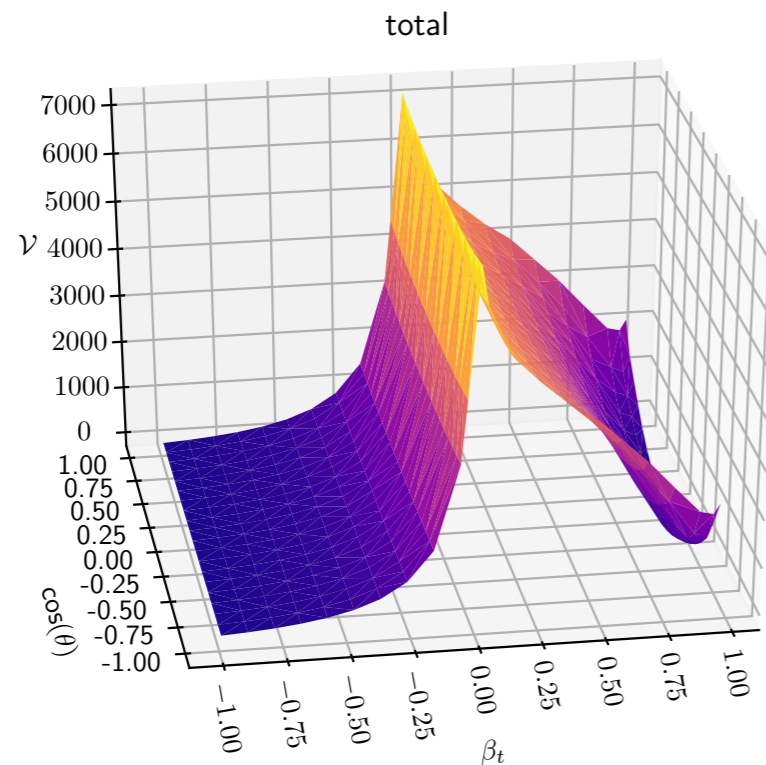


**Interpolated  
surface  
(visualisation)**

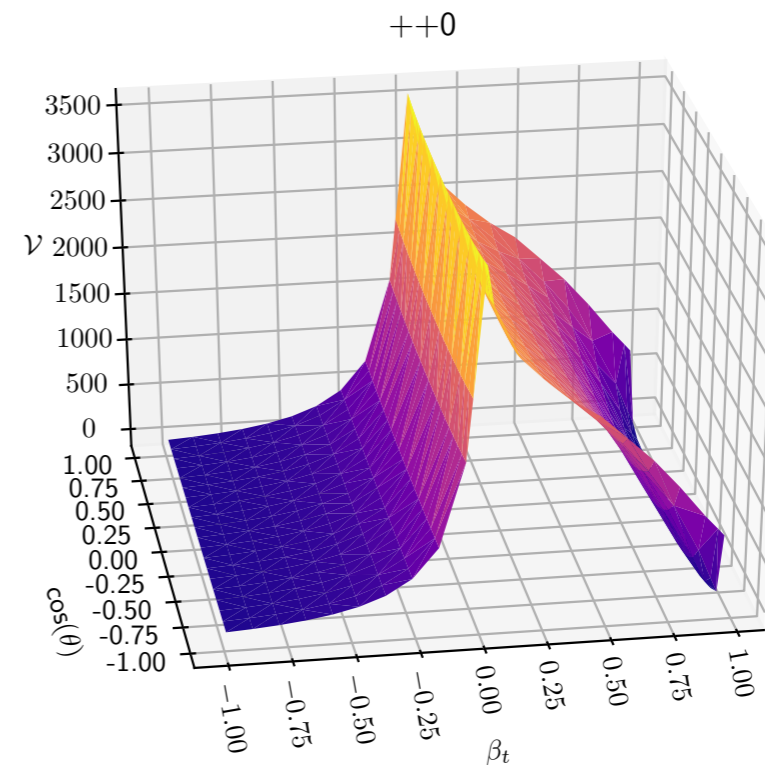


# Amplitude Result

Observe that modes with longitudinally polarised Z boson dominate total

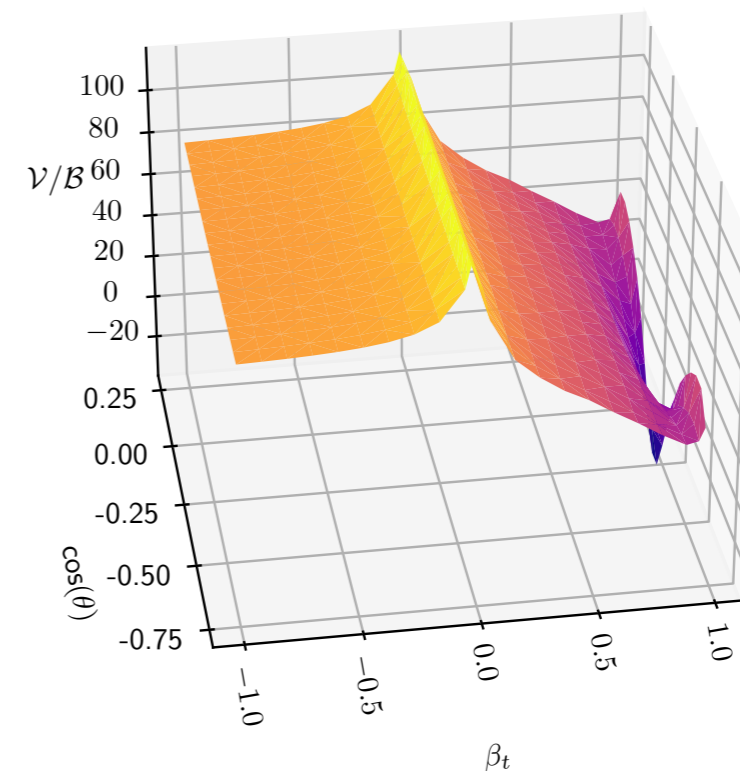


$\sim 2 \times$



Ratio between Born squared amplitude and Born-Virtual interference not flat

**Reminder:** plot missing real contribution (so plot is not NLO/LO 'K-factor')

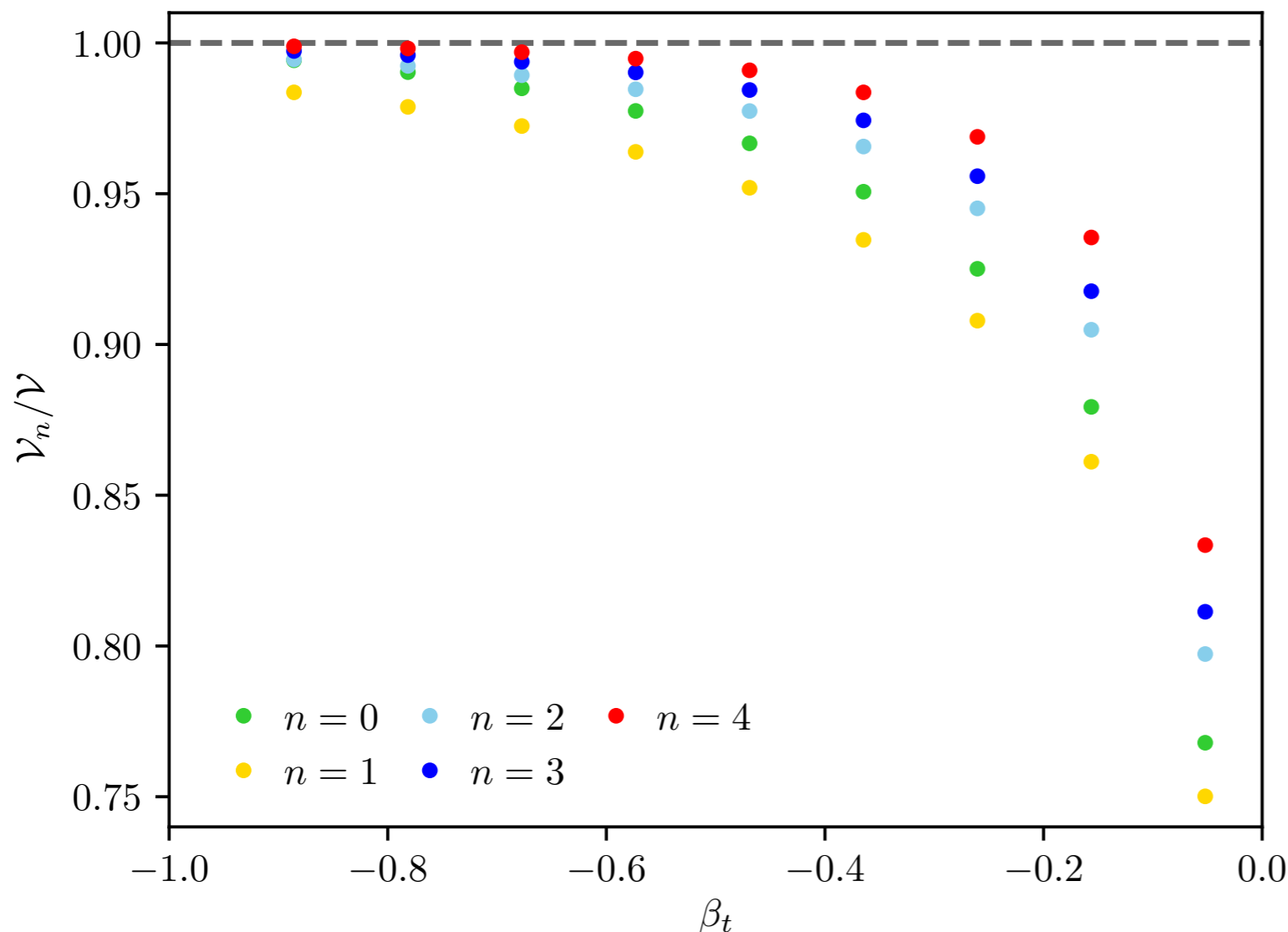


# Comparison to Large $m_t$ Expansion

The amplitude has been expanded around large- $m_t$  and computed analytically  
 Hasselhuhn, Luthe, Steinhauser 17; Davies, Mishima, Steinhauser 20

Let us compare our result to the Born  
 reweighted  $1/m_t^{2n}$  expansion:

$$\mathcal{V}_n = \frac{\mathcal{B}}{\mathcal{B}_n} \tilde{\mathcal{V}}_n + \mathcal{V}^{1\text{PR}}$$



Per mille level agreement far  
 below top quark threshold:

$$\mathcal{V}_4/\mathcal{V} = 0.9989$$

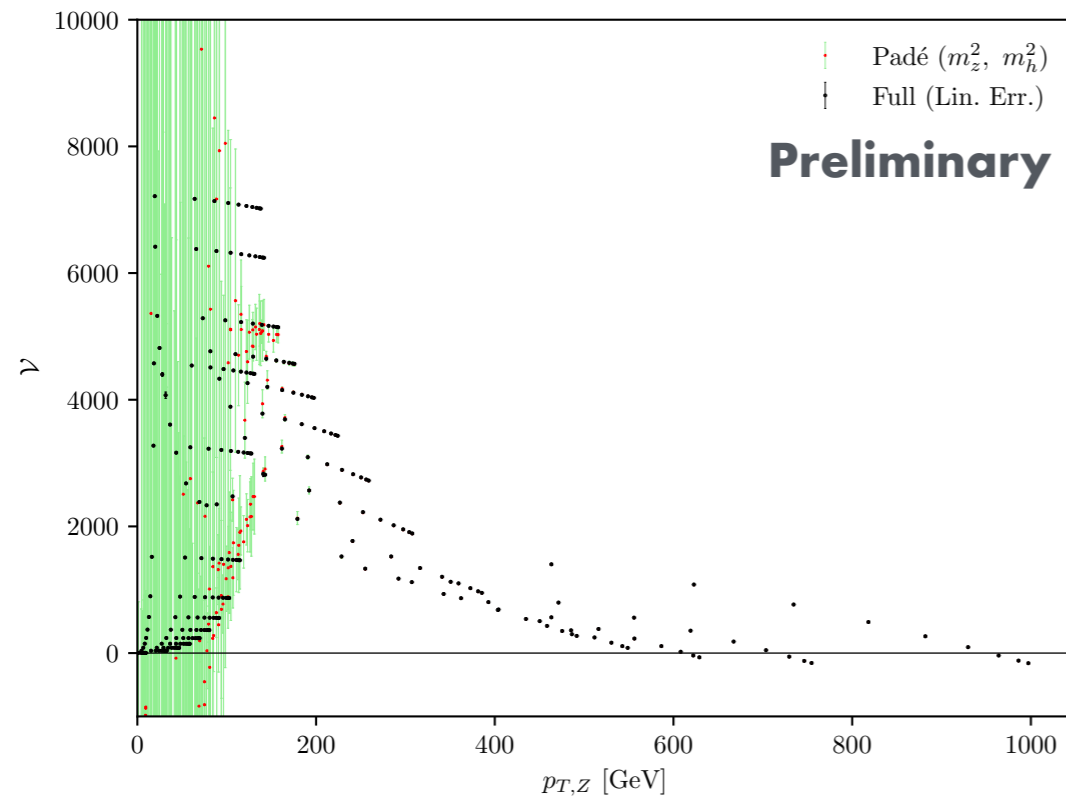
Expansion breaks down at  
 threshold, observe that it  
 differs from our result

Observation:  $n = 1$  apparently  
 worse than  $n = 0$

# Comparison to Small $m_t$ Expansion

The amplitude has also been expanded around small  $m_t, m_h, m_z$

Davies, Mishima, Steinhauser 20; Mishima 18

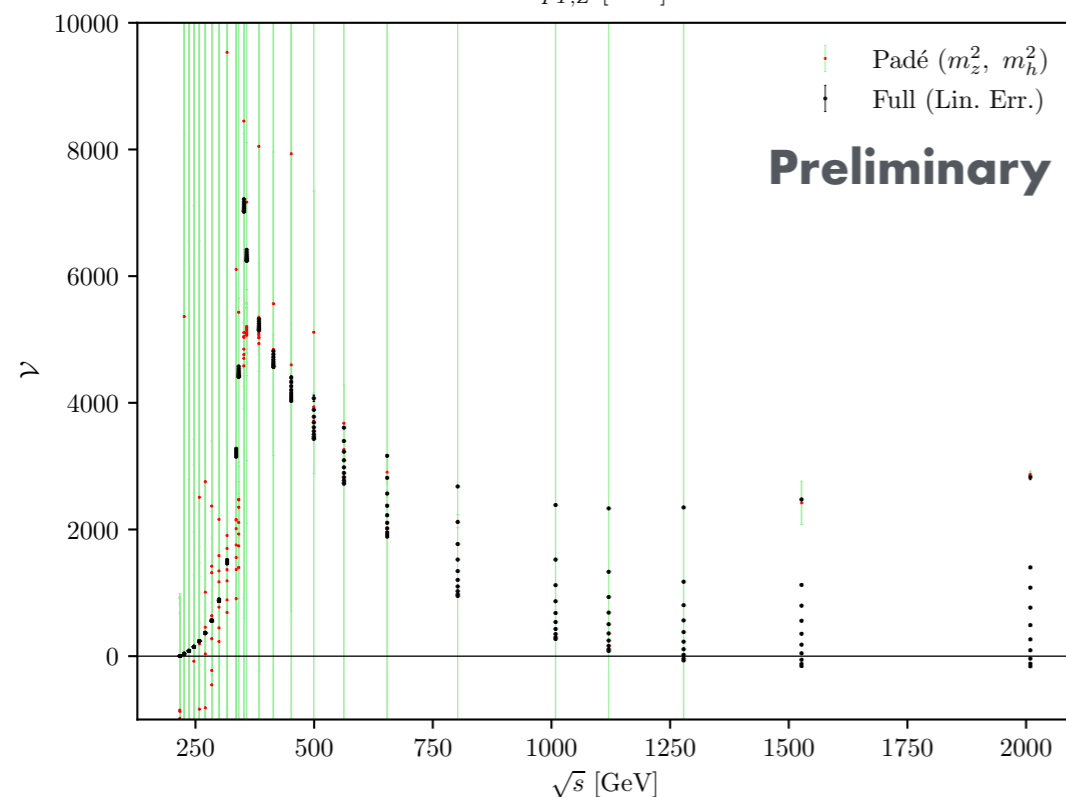


Agreement with Padé improved  
expanded result  $\mathcal{O}(m_z^2, m_h^2, m_t^{32})$

$\sim 2\%$  level for  $p_T \gtrsim 225$

$\sim 10\%$  level for  $150 < p_T < 225$

Consistent with Padé/full at LO level



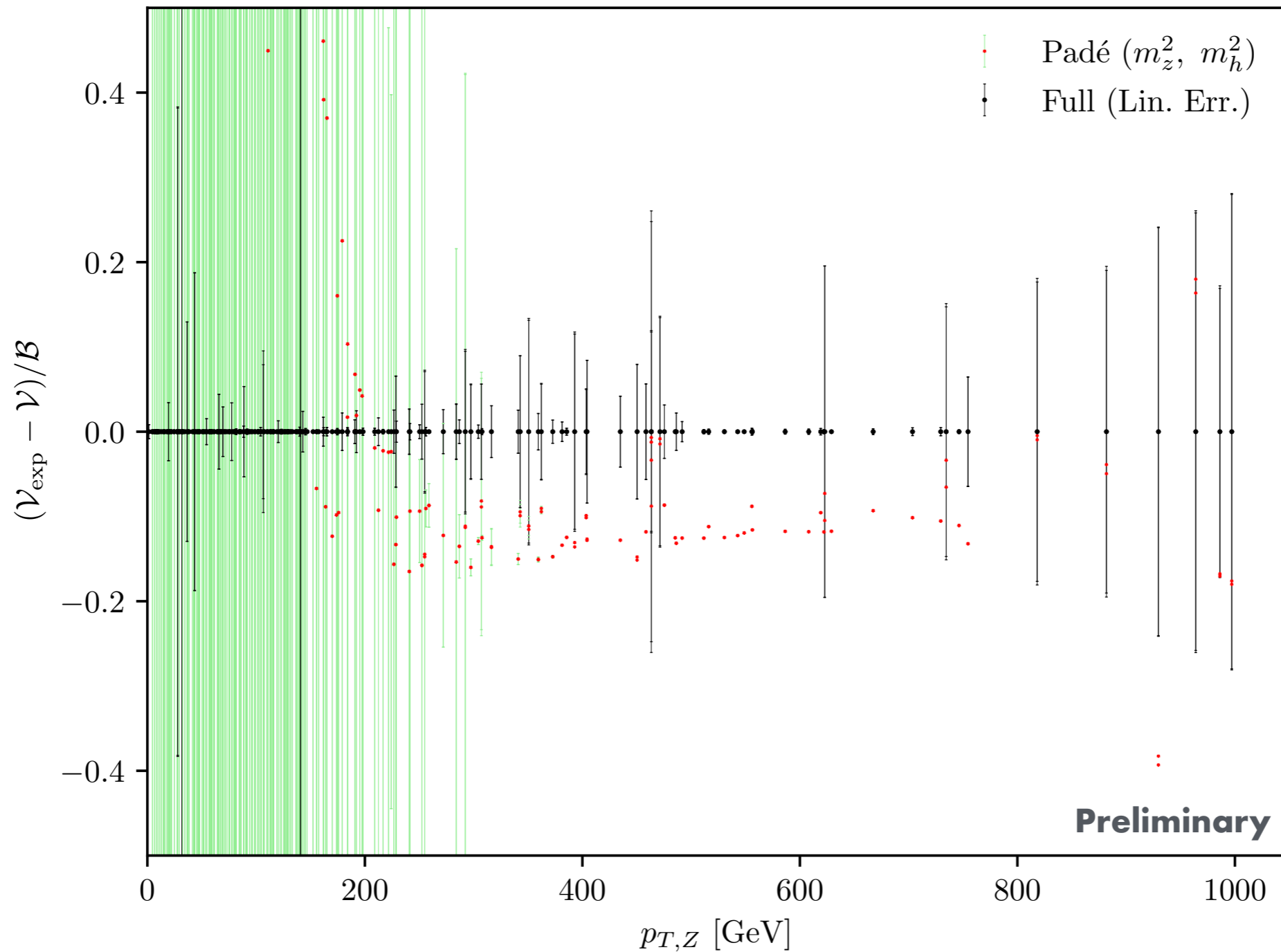
Not all points agreeing well even for  
large  $\sqrt{s}$

Convergence of the Padé result  
depends on  $m_T \ll s, |t|, |u|$  can have  
small  $|t|$  even for large  $s$  (if  $p_T$  is small)



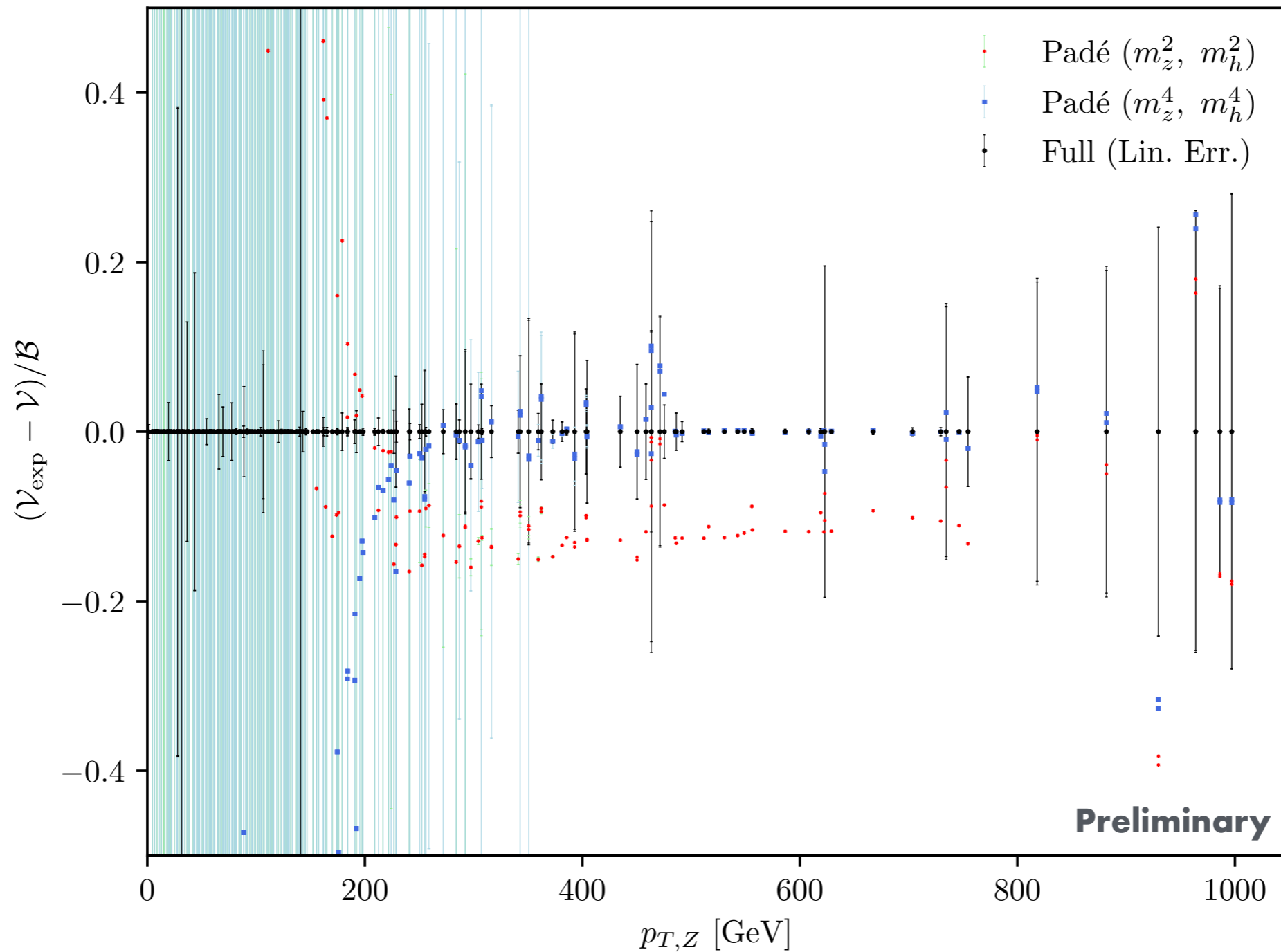
# Comparison to Small $m_t$ Expansion (II)

Can the Padé result be improved by including terms of order  $m_z^4$ ,  $m_h^4$ ?



# Comparison to Small $m_t$ Expansion (II)

Can the Padé result be improved by including terms of order  $m_z^4$ ,  $m_h^4$ ?



New Padé terms provided by: Davies, Mishima, Steinhauser

Now find **excellent** agreement for  $p_T \geq 200$  GeV

# Comparison to Expansion (Small $m_h, m_z$ )

Can expand in only  $m_h, m_z$  and retain full  $m_t$  dependence Wang, Xu, Xu, Yang 21

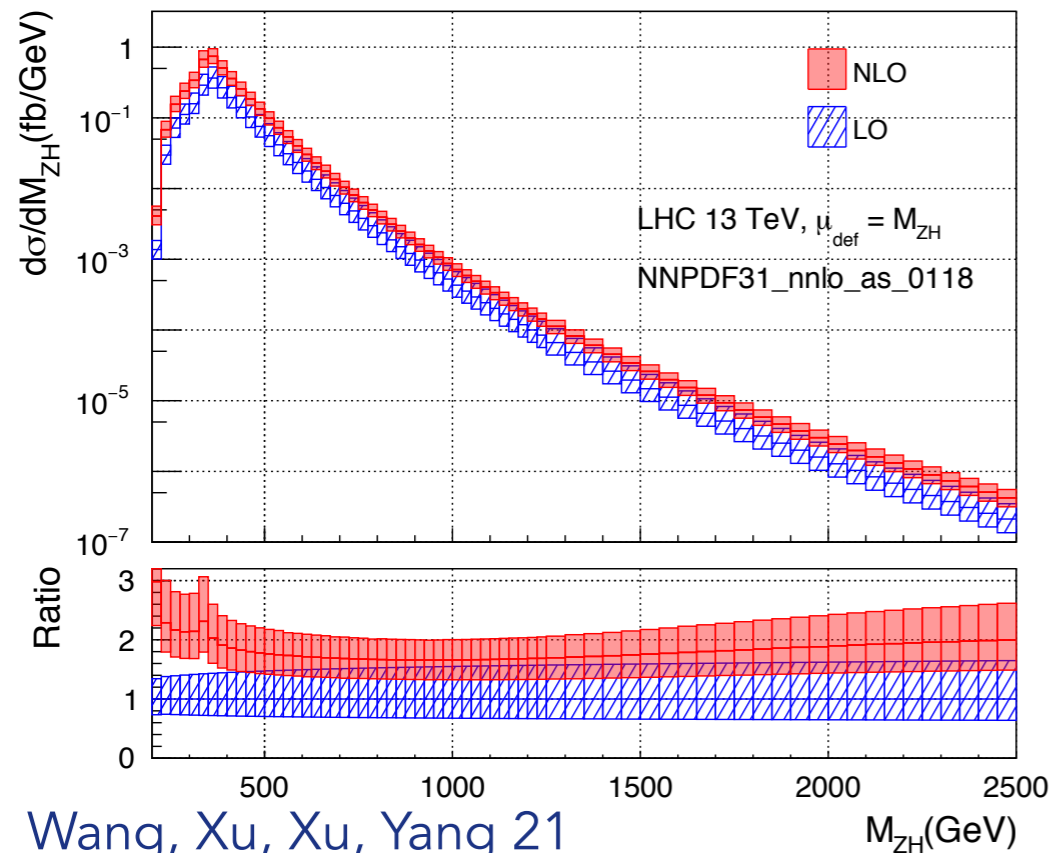
Integrals appearing in the expansion (scales  $s, t, m_t^2$ ) are known

Caron-Huot, Henn 14; Becchetti, Bonciani 18; Xu, Yang 18; Wang, Wang, Xu, Xu, Yang 20;

Expansion shows good agreement with numerical result in most (all?) phase-space regions

No breakdown near top threshold

$\hat{s}/m_t^2$	$\hat{u}/m_t^2$	$\mathcal{V}'_{\text{fin}}$			
		pySecDec	$\mathcal{O}(m^0)$	$\mathcal{O}(m^2)$	$\mathcal{O}(m^4)$
1.707133657190554	-0.441203767016323	35.429092(6)	35.9823	35.5530	35.4478
3.876056604162662	-1.616287256345735	4339.045(1)	4319.37	4336.63	4338.73
4.130574250302561	-1.750372271104745	6912.361(3)	6870.47	6906.92	6911.64
4.130574250302561	-2.595461551488002	6981.09(2)	6979.28	6980.14	6980.85
134.5142052093564	-70.34125943305149	-153.9(4)	-154.543	-154.458	-154.460
134.5142052093564	-105.1770655376327	527(4)	524.585	525.958	525.965



Authors published NLO results for  $gg \rightarrow ZH$

**Virtuals:** small  $m_h, m_z$  expansion

**Reals:** GoSam Cullen et al.

Gives stable invariant mass distribution, sizeable corrections  $\sim$ LO (as expected)

# Conclusion

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## We have entered the precision Higgs era

- Over coming years, expect greater demand for precise theory predictions (required to exploit experimental measurements)
- Detailed searches for deviations, e.g: differential measurements, constraining EFT couplings, off-shell measurements, ...

## I have presented a calculation which underscores the usefulness of

- Numerical methods for solving Feynman integrals (**new pySecDec out now!**)

## Next steps...

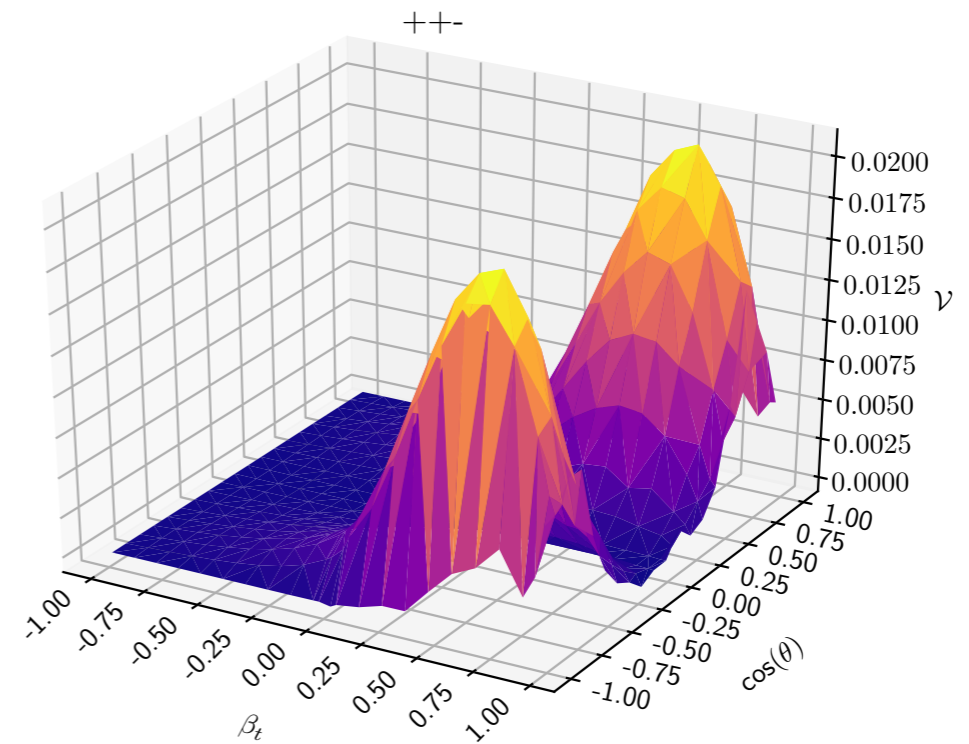
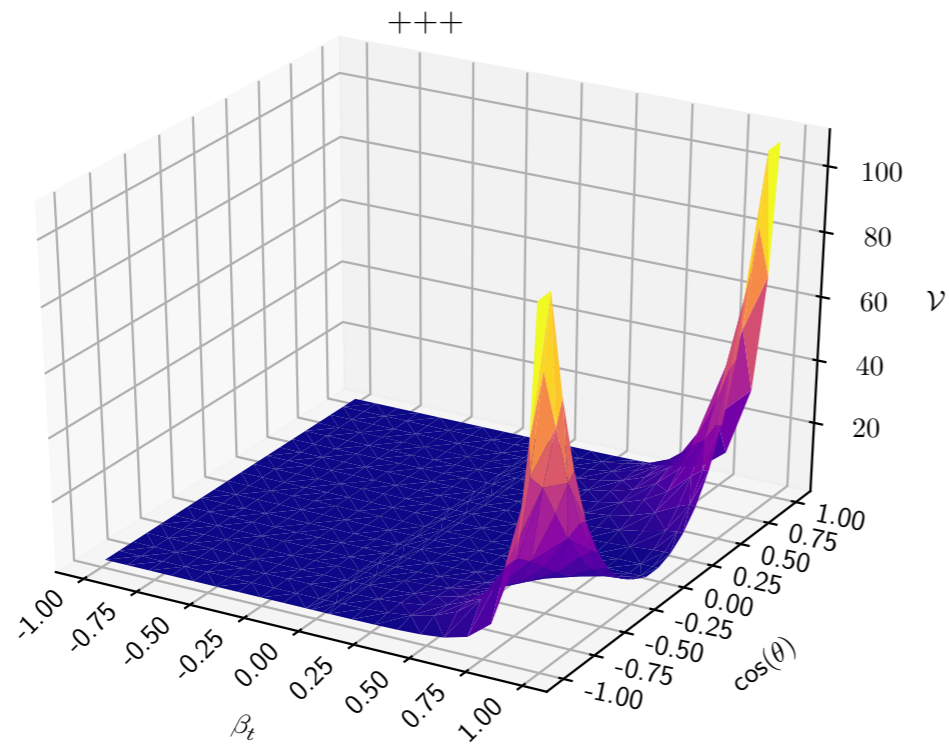
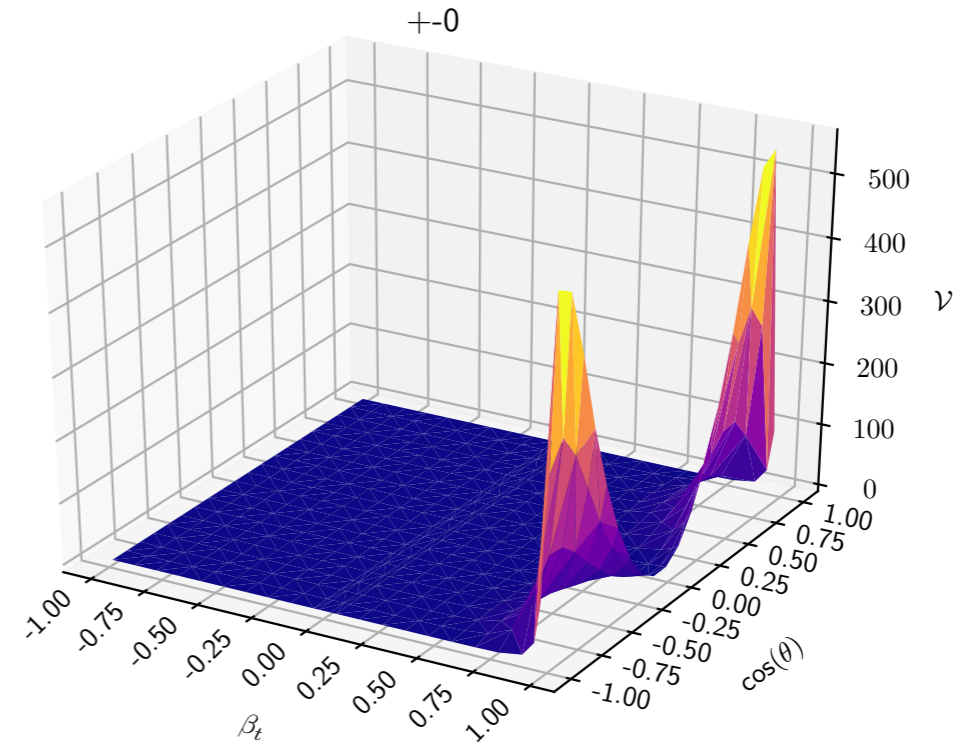
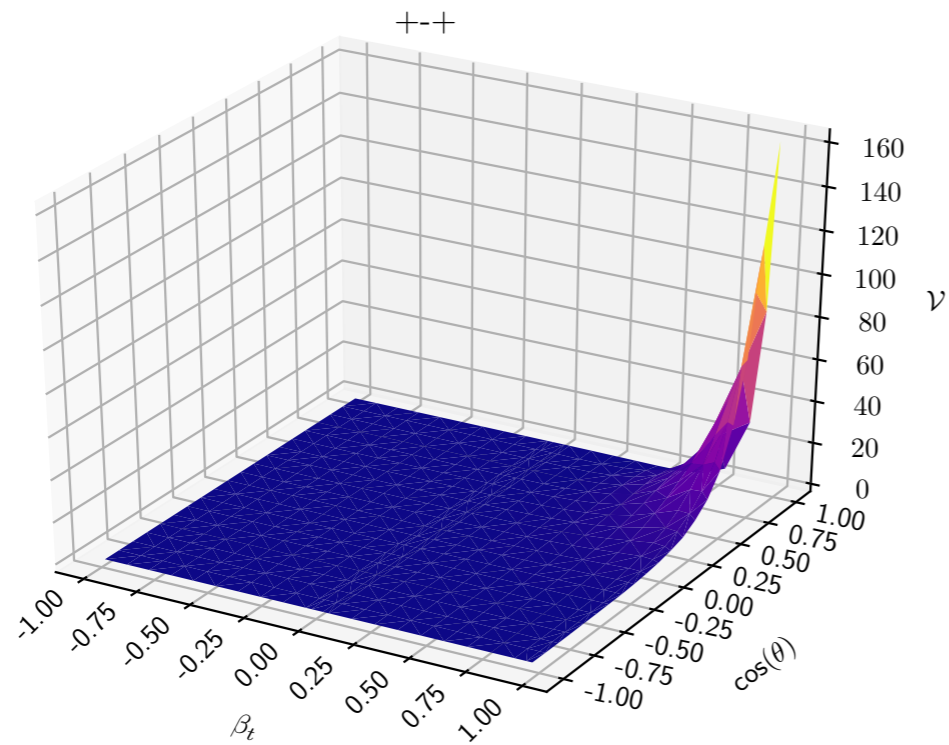
- Put the pieces together in order to obtain complete NLO results
- Incorporate into public tools for  $pp \rightarrow ZH$  (?)

**Thank you for listening!**

Backup

# Helicity Amplitudes

We can produce precise results for all helicity amplitudes also in kinematic limits!



# Decomposition: $gg \rightarrow ZH$

**Idea:** construct projectors for linearly polarised amplitudes in c.o.m frame, directly compute polarised amplitudes [Chen 19](#)

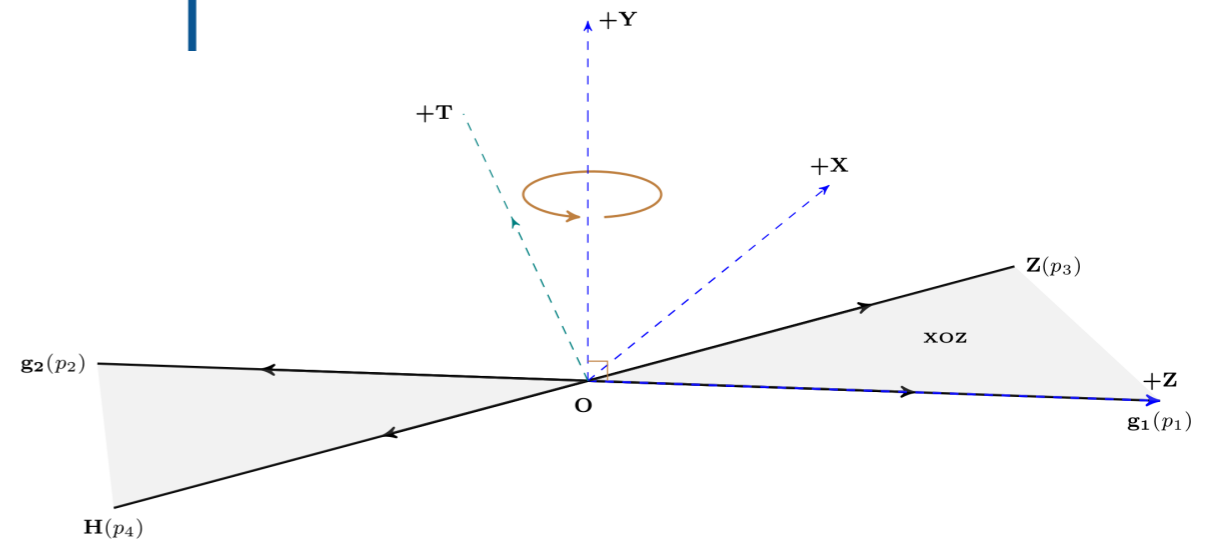
Polarisation vectors can be expressed (up to normalisation factors  $\mathcal{N}_i$ ) in terms of external momenta:

$$\begin{aligned}\varepsilon_x^\mu &= \mathcal{N}_x (-s_{23}p_1^\mu - s_{13}p_2^\mu + s_{12}p_3^\mu) \\ \varepsilon_y^\mu &= \mathcal{N}_y (\epsilon_{\mu_1 \mu_2 \mu_3}^\mu p_1^{\mu_1} p_2^{\mu_2} p_3^{\mu_3}) \\ \varepsilon_T^\mu &= \mathcal{N}_T \left( (-s_{23}(s_{13} + s_{23}) + 2m_z^2 s_{12}) p_1^\mu + \right. \\ &\quad \left. (s_{13}(s_{13} + s_{23}) - 2m_z^2 s_{12}) p_2^\mu + s_{12}(-s_{13} + s_{23}) p_3^\mu \right) \\ \varepsilon_l^\mu &= \mathcal{N}_l (-2m_z^2 (p_1^\mu + p_2^\mu) + (s_{13} + s_{23}) p_3^\mu)\end{aligned}$$

$$\begin{aligned}\varepsilon_x \cdot \{p_1, p_2\} &= 0 \\ \varepsilon_y \cdot \{p_1, p_2\} &= 0 \\ \{\varepsilon_y, \varepsilon_T, \varepsilon_l\} \cdot p_3 &= 0 \\ \varepsilon_i^2 &= -1\end{aligned}$$

**Projectors** are just products of pol. vecs.

$$\begin{aligned}\mathcal{P}_1^{\mu_1 \mu_2 \mu_3} &= \varepsilon_x^{\mu_1} \varepsilon_x^{\mu_2} \varepsilon_y^{\mu_3} & \mathcal{P}_2^{\mu_1 \mu_2 \mu_3} &= \varepsilon_x^{\mu_1} \varepsilon_y^{\mu_2} \varepsilon_T^{\mu_3}, \\ \mathcal{P}_3^{\mu_1 \mu_2 \mu_3} &= \varepsilon_x^{\mu_1} \varepsilon_y^{\mu_2} \varepsilon_l^{\mu_3} & \mathcal{P}_4^{\mu_1 \mu_2 \mu_3} &= \varepsilon_y^{\mu_1} \varepsilon_x^{\mu_2} \varepsilon_T^{\mu_3}, \\ \mathcal{P}_5^{\mu_1 \mu_2 \mu_3} &= \varepsilon_y^{\mu_1} \varepsilon_x^{\mu_2} \varepsilon_l^{\mu_3} & \mathcal{P}_6^{\mu_1 \mu_2 \mu_3} &= \varepsilon_y^{\mu_1} \varepsilon_y^{\mu_2} \varepsilon_y^{\mu_3}.\end{aligned}$$



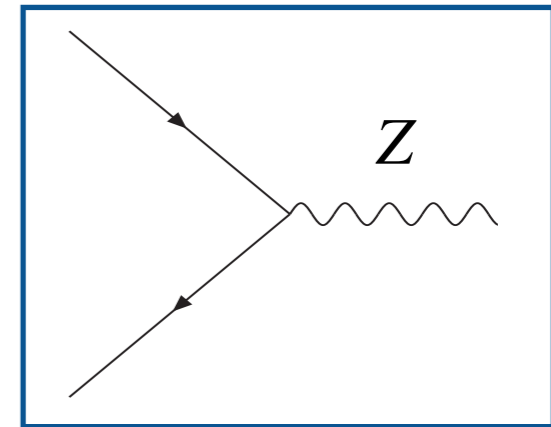
Cross checked with conventional form factor decomposition at LO and at NLO with expansions [Davies, Mishima, Steinhauser 20](#)

# Dimensional Regularisation & $\gamma_5$

## Z-Fermion Vertex

Contains vector  $\sim v_t \gamma_\mu$  and axial-vector  $\sim a_t \gamma_\mu \gamma_5$ :

$$\mathcal{V}_\mu^{Vf\bar{f}} = i \frac{e}{2 \sin \theta_W \cos \theta_W} \gamma_\mu (v_t + a_t \gamma_5)$$



We use dimensional regularisation ( $d = 4 - 2\epsilon$ ) to regulate divergences appearing in loop integrals, however, one can't retain all properties of  $\gamma_5$  in  $d \neq 4$  dimensions

## Larin Scheme (ZH, ZZ)

Sacrifice anti-commuting property of  $\gamma_5$

$$J_\mu^5 = Z_{5,ns} \quad J_{\mu,B}^5 = Z_{5,ns} \left[ \frac{i}{3!} \epsilon_{\mu\nu\rho\sigma} \bar{\psi} \gamma^\nu \gamma^\rho \gamma^\sigma \psi \right]$$

$$P^5 = Z_{5,p} \quad P_B^5 = Z_{5,p} \left[ \frac{i}{4!} \epsilon_{\mu\nu\rho\sigma} \bar{\psi} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \psi \right]$$

Fix Ward identities/ABJ anomaly:

$$Z_{5,ns} = 1 + \alpha_s (-4C_F) + \dots$$

$$Z_{5,p} = 1 + \alpha_s (-8C_F) + \dots$$

Larin, Vermaseren 91; Larin 93

Alternative schemes exist e.g:

## Kreimer Scheme (ZZ)

Retain  $\{\gamma_5, \gamma^\mu\} = 0$ , but, sacrifice cyclicity of traces involving  $\gamma_5$

Define 'reading point' and carefully manipulate all traces

Kreimer 90; Korner, Kreimer, Schilcher 92

Used in our calculation of  $gg \rightarrow ZZ$

Agarwal, SPJ, von Manteuffel 20




# Reduction

---

Integration by parts Identities:

$$\int d^d k_1 \cdots d^d k_l \frac{\partial}{\partial k_i^\mu} [v^\mu I(k_1, \dots, k_l; p_1, \dots, p_m)] = 0$$

 **loop/external momentum**

Produce linear relations between integrals [Tkachov 81](#); [Chetyrkin 81](#)

Can perform e.g. Gaussian elimination on system of equations

Relate integrals to a smaller set (**basis**) of **Master integrals**

The choice of basis impacts:

- 1) **Complexity of the coefficients in the amplitude**
- 2) **Difficulty of computing the integrals**

Always possible to pick a basis of finite integrals using:

- Dimension Shifts [Tarasov 96](#); [Lee 10](#)
- Dots
- Numerator Insertions (*optional, not used for gg → ZH*)

[Panzer 14](#);  
[von Manteuffel, Panzer,](#)  
[Schabinger 15](#)

The finite basis greatly improves numerical performance

# Reduction (II)

Need tools to actually solve these systems of equations...

## ZZ Computation

FinRed von Mantueffel (Private)  
+ Syzygy Solver Agarwal, von Mantueffel

**Master Integrals: 264**

## ZH Computation

Kira 2 + FireFly Maierhöfer, Usovitsch, Uwer 18;  
Klappert, Lange, P. Maierhöfer,  
Usovitsch 20; Klappert, Lange  
20; Klappert, Klein, Lange 20

**Master Integrals: 452**

Both toolchains extensively rely on the use of finite fields

See e.g: von Mantueffel, Schabinger 14; Peraro 16

Even with these tools, still too difficult to obtain fully symbolic amplitudes

Fix mass ratios ZZ:  $\frac{m_z^2}{m_t^2} = \frac{5}{18}$  and ZH:  $\frac{m_z^2}{m_t^2} = \frac{23}{83}$ ,  $\frac{m_H^2}{m_t^2} = \frac{12}{23}$

# Master Integral Basis ( $gg \rightarrow ZH$ )

---

**To select our master integrals, we took the following pragmatic approach:**

- 1) Consider quasi-finite integrals (prefer finite integrals)

$$I = \frac{I_{-2}}{\epsilon^2} + \frac{I_{-1}}{\epsilon} + I_0 + \dots \quad \rightarrow \quad I' = I'_0 + \dots$$

- 2) Choose a basis in which the  $d$ -dependence of denominators factorises from the kinematic dependence (in practice we achieve this by brute force neglecting subsectors, public tools are available [Smirnov, Smirnov 20](#); [Usovitsch 20](#))

$$\frac{N(s, t, d)}{D(s, t, d)} I + \dots \rightarrow \frac{N'(s, t, d)}{D'_1(d)D'_2(s, t)} I' + \dots$$

- 3) Prefer simple denominator factors
- 4) Prefer computing fewer orders in epsilon for each master (found a basis in which all 7-propagator integrals start contributing only at  $\epsilon^{-1}$ )
- 5) Prefer simpler numerators (check number of terms/file size)

See also: Matthias Kerner, *Loops and Legs Proceedings 2018*

Steps 2-5 reduced the size of amplitude by factor of 5

Largest coefficient (double-tadpole) 150 MB  $\rightarrow$  5 MB

# Amplitude Evaluation (IV)

A peak behind the curtain (enabled by setting verbose=True)

```
#
# Compute a first estimate of each integral (n: 50789 x 32 samples of integral)
# Note: each order of each sector is computed separately (and can be known to a different precision)
#
computing integrals to satisfy mineval 50000
integral 1/16: bubble_u_sector_1_order_0, time: 0.0 s res: (0,0) +/- (0,0) -> (1,0) +/- (8.89904e-17,0), n: 0 -> 50789
integral 2/16: bubble_u_sector_1_order_1, time: 0.0 s res: (0,0) +/- (0,0) -> (2.22314,0) +/- (1.9927e-15,0), n: 0 -> 50789
integral 3/16: bubble_t_sector_1_order_0, time: 0.0 s res: (0,0) +/- (0,0) -> (1,0) +/- (9.00691e-17,0), n: 0 -> 50789
integral 4/16: bubble_t_sector_1_order_1, time: 0.0 s res: (0,0) +/- (0,0) -> (1.73764,0) +/- (2.19938e-15,0), n: 0 -> 50789
...

#
# Estimate amplitude(s) using integral results
#
amplitude0 = + ((0,0) +/- (2.41174e-16,0))*eps^-1 + ((-28.4316,-1.6741e-09) +/- (4.06609e-09,2.39249e-09)) + 0(eps)

#
# Examine contribution of each integral to err. of amp. and estimate how many samples we need (n: known -> required)
# Note: not all sectors will be recomputed, different sectors will be computed to different precisions
#
sum: sum_eps^0, term: WINTEGRAL, integral 5: box_6_sector_1_order_0, current integral result: (0.478203,4.5158e-11) +/-
(2.31205e-10,4.72335e-11), contribution to sum error: 2.0946e-09, increase n: 50789 -> 968960972
sum: sum_eps^0, term: WINTEGRAL, integral 15: box_8_sector_5_order_0, current integral result: (0.0173611,-5.39441e-13) +/-
(3.16251e-12,1.29608e-12), contribution to sum error: 1.64054e-10, increase n: 50789 -> 193374172
...

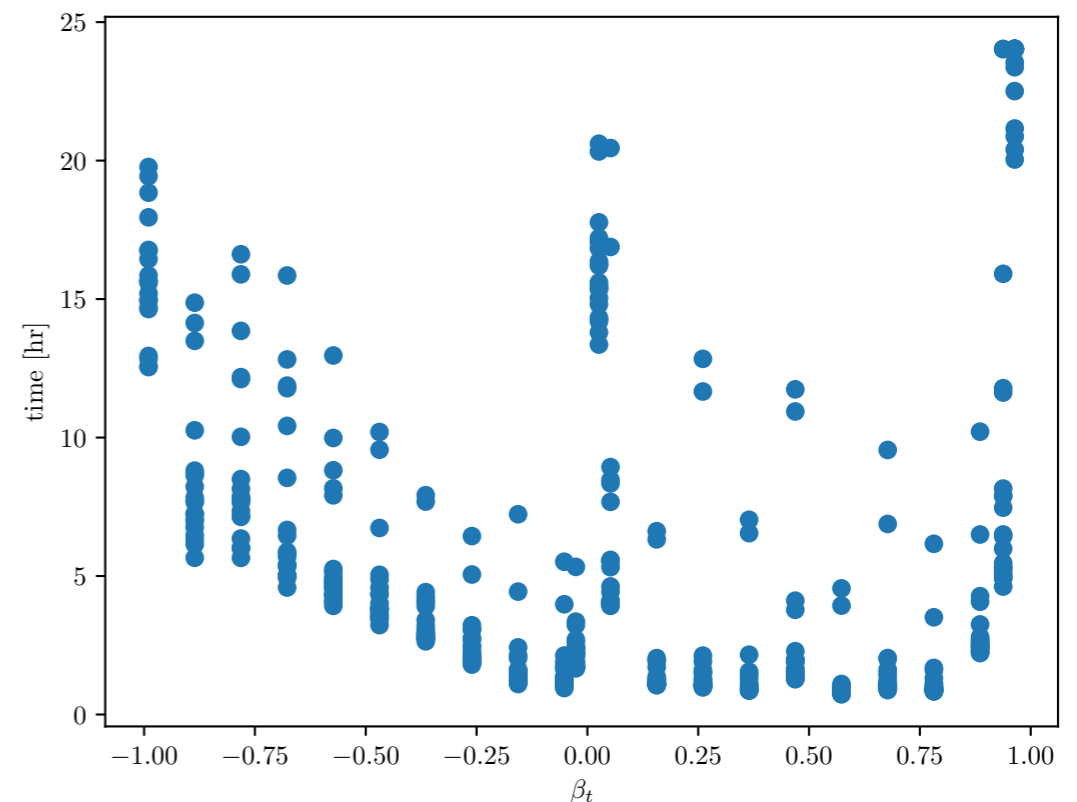
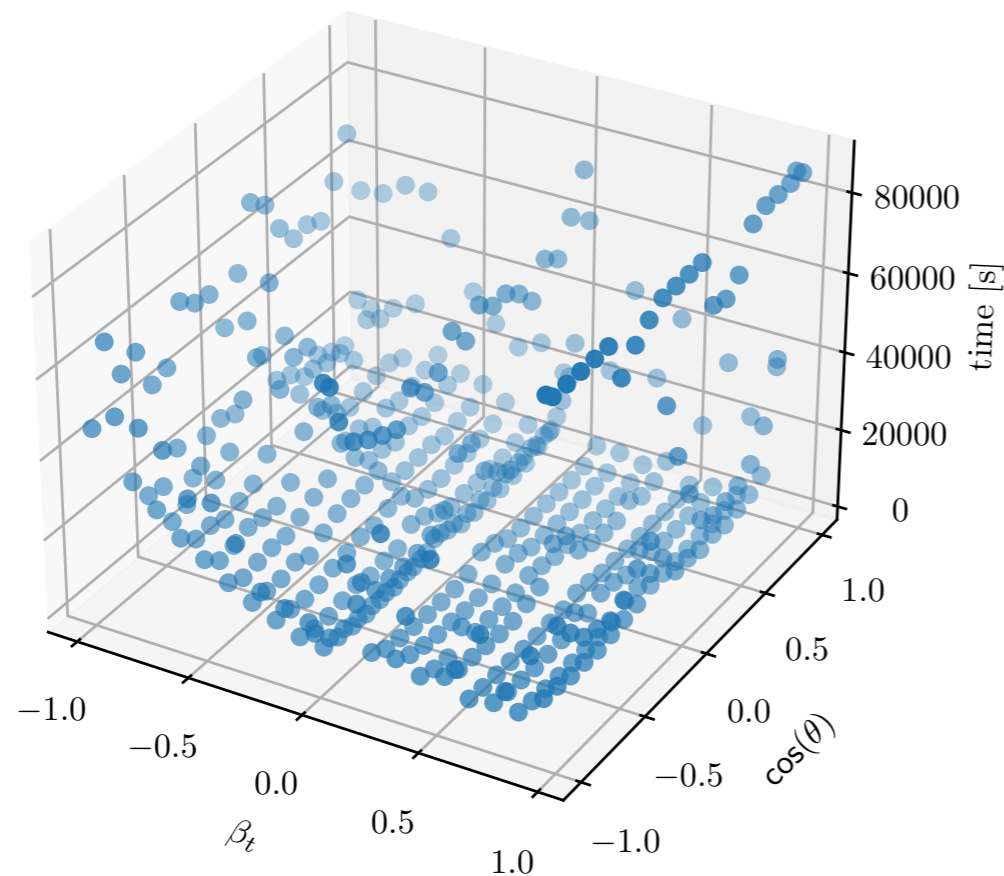
#
# Iterate until we obtain the desired precision
# Note: reason for iteration is printed (long running/run away jobs can be debugged straightforwardly)
#
run further refinements: true
computing integrals to satisfy error goals on sums: epsrel 1e-14, epsabs 1e-14
...
```

# Evaluation of the Amplitude (Timing)

Each phase-space point evaluated with 2 x Nvidia Tesla V100 GPUs  
Precision goal set to 0.3% for each (linearly polarised) amplitude

## Timing/ point:

**Min:** 45 mins,    **Max:** 24 hr (wall-clock), ~65 hr (high-energy),    **Median:** 3.5 hr



Worst performance near to  $ZH, t\bar{t}$  thresholds, high-energy and forward scattering

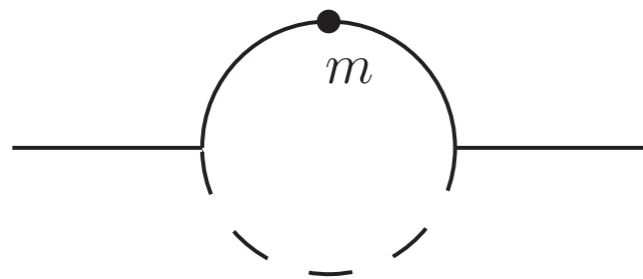
# Expansion by Regions: Momentum Space

---

# Expansion by Regions: Bubble Example

Let us consider the large momentum limit  $|p|^2 \gg m^2$  of some integral, we therefore want to expand in the small dimensionless ratio  $m^2/p^2$

**Example:** (finite) 1-loop bubble integral [Jantzen 2011](#)



$$G = \mu^{2\epsilon} \int \frac{d^D k}{i\pi^{D/2}} \frac{1}{(k+p)^2(k^2-m^2)^2}$$

$D = 4 - 2\epsilon$

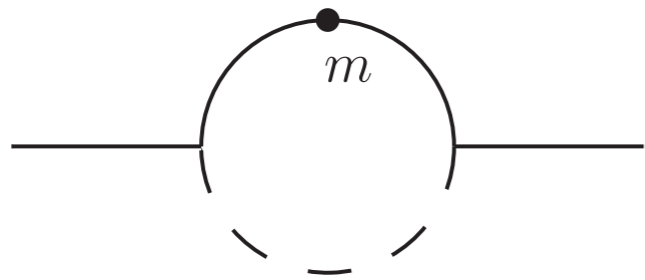
If we can compute the integral, the expansion after integration is straightforward

$$G = \frac{1}{p^2} \left[ \ln \left( \frac{-p^2 - i0}{m^2} \right) + \ln \left( 1 - \frac{m^2}{p^2} \right) \right] + \mathcal{O}(\epsilon)$$

$$= \frac{1}{p^2} \left[ \ln \left( \frac{-p^2 - i0}{m^2} \right) - \sum_{j=1}^{\infty} \frac{1}{j} \left( \frac{m^2}{p^2} \right)^j \right] + \mathcal{O}(\epsilon)$$

Now let's try to expand before integration

# Expansion by Regions: Bubble Example (II)



$$G = \int \mathbf{D}k I = \mu^{2\epsilon} \int \frac{d^D k}{i\pi^{D/2}} \frac{1}{(k+p)^2 (k^2 - m^2)^2}$$

Since  $|p^2| \gg m^2$  we may start by expanding the 2nd propagator around small  $m^2$ :

$$I^{(h)} = \sum_i T_i^{(h)} I = \frac{1}{(k+p)^2} \left( \frac{1}{(k^2)^2} + 2 \frac{m^2}{(k^2)^3} + \dots \right)$$

Integrating the expansion over the **whole domain**  $k \in \mathbb{R}^d$  we get:

$$G^{(h)} = \sum_i T_i^{(h)} G = \frac{1}{p^2} \left[ -\frac{1}{\epsilon} + \ln \left( \frac{-p^2 - i0}{\mu^2} \right) - \sum_{j=1}^{\infty} \frac{2}{j} \left( \frac{m^2}{p^2} \right)^j \right] + \mathcal{O}(\epsilon)$$

Here, we implicitly assumed  $k \gg m^2$  and neglected the region where  $k \sim m$ , let us compute this region too...



# Expansion by Regions: Bubble Example (III)

---

Expanding the 1st propagator around large  $p^2$ :

$$I^{(s)} = \sum_i T_i^{(s)} I = \frac{1}{(k^2 - m^2)^2} \left( \frac{1}{p^2} - \frac{k^2 + 2p \cdot k}{(p^2)^2} + \dots \right)$$

Integrating the expansion over the **whole domain**  $k \in \mathbb{R}^d$  we get:

$$G^{(s)} = \sum_i T_i^{(s)} G = \frac{1}{p^2} \left[ \frac{1}{\epsilon} + \ln \left( \frac{\mu^2}{m^2} \right) + \sum_{j=1}^{\infty} \frac{1}{j} \left( \frac{m^2}{p^2} \right)^j \right] + \mathcal{O}(\epsilon)$$

Summing the **hard (h)** and **soft (s)** regions we get:

$$G = G^{(h)} + G^{(s)} = \frac{1}{p^2} \left[ \ln \left( \frac{-p^2 - i0}{m^2} \right) - \sum_{j=1}^{\infty} \frac{1}{j} \left( \frac{m^2}{p^2} \right)^j \right] + \mathcal{O}(\epsilon)$$

**This reproduces the expanded result**, but why does this work?

- 1) Did we not **double-count** when replacing  $\int Dk \rightarrow \int Dk I^{(h)} + \int Dk I^{(s)}$  ?
- 2) How do we **choose the regions**?

# Expansion by Regions: Bubble Example (IV)

---

1) Did we not double-count when replacing  $\int Dk \rightarrow \int Dk I^{(h)} + \int Dk I^{(s)}$  ?

This example (and several others) was examined in great detail by Jantzen, he noted: Jantzen 2011

The expansions  $\sum_i T_i^{(h)}$ ,  $\sum_i T_i^{(s)}$  converge absolutely in their respective domains

$$D_h = \{k \in \mathbb{R}^d : |k^2| \geq \Lambda^2\}$$

$$D_s = \{k \in \mathbb{R}^d : |k^2| < \Lambda^2\}$$

with  $m^2 \ll \Lambda^2 \ll |p^2|$

The expansions commute  $T_i^{(h)} T_j^{(s)} I = T_j^{(s)} T_i^{(h)} I = T_{i,j}^{(h,s)} I$

$$\text{Thus } G = \sum_i \int_{k \in D_h} Dk T_i^{(h)} I + \sum_j \int_{k \in D_s} Dk T_j^{(s)} I = G^{(h)} + G^{(s)} - G^{(h,s)}$$

Finally, the overlap/multiple expansion contribution  $G^{(h,s)}$  turns out to be **scaleless (=0)**, in dimensional regularisation such integrals vanish, **we did not double-count!**

# Expansion by Regions in pySecDec

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# Geometric Method: Scaleless Integrals

---

## Momentum space

In dimensional regularisation, **scaleless integrals are 0**

$$G(\{k_i\}_a, \{ck_i\}_b) = c^{N_G} G(\{k_i\}) \implies G(k_i) = 0, \quad \{k_i\} = \{k_i\}_a \cup \{k_i\}_b$$

Where  $G(\{k_i\})$  is a Feynman integral depending on loop momenta  $\{k_i\}$ ,  $c \neq 0$  and  $N_G$  is some scaling dimension

## Feynman parameter space

$$(\mathcal{U} \times \mathcal{F})(c^{\mathbf{v}} \mathbf{x}) = c^N (\mathcal{U} \times \mathcal{F})(\mathbf{x}), \quad \mathbf{v} \neq n\mathbf{1}, \quad n \in \mathbb{R}$$

## Geometrical viewpoint

For  $\Delta$  built from  $\mathcal{U} + \mathcal{F}$

$$\dim(\Delta) = \dim(\mathbf{x}) \iff G \text{ scaleful}$$

$$\dim(\Delta) < \dim(\mathbf{x}) \iff G \text{ scaleless}$$

This was also used in earlier works on EBR [Pak, Smirnov 10](#)

# Geometric Method: Overlap Contributions

---

Jantzen showed that under some quite general conditions [Jantzen 2011](#)

$$G = \sum_{f \in F^+} G^{(f)} - \sum_{\{f_1, f_2\} \subset F^+}^{\langle F_c^+ + 1 \rangle} G^{(f_1, f_2)} + \dots - (-1)^n \sum_{\{f_1, \dots, f_n\} \subset F^+}^{\langle F_c^+ + 1 \rangle} G^{(f_1, \dots, f_n)} + \dots + (-1)^{N_c} \sum_{f' \in F_{nc}^+} G^{(f', f_1, \dots, f_{N_c})}$$

---

## overlap contributions / multiple expansions

Where  $F_c^+$  yield commuting expansions,  $F_{nc}^+$  non-commuting expansions and the sums  $\{f_1, \dots\}$  run over subsets containing at most one region from  $F_{nc}^+$

However, for **regulated integrals** (dim reg + analytic regulators) **these multiple expansions usually vanish**

We always neglect them in our code, but one can easily check this case-by-case

**Reason:** Consider Newton polytope with  $\dim(\Delta) = \dim(\mathbf{x}) + 1$

- 1st expansion: picks terms forming a facet  $f_1$ ,  $\dim(f_1) = \dim(\mathbf{x}) \implies$  scaleful
- 2nd expansion: picks out terms that are an "intersection" between two facets  $f_{1,2}$ ,  $\dim(f_{1,2}) = \dim(\mathbf{x}) - 1 \implies$  scaleless (unless facets are parallel)

# Geometric Method: Additional Regulators

**Issue 1:** EBR can introduce spurious singularities that are not regulated by dim reg.

Let  $\nu$  be a vector of propagator powers,  $D = 4 - 2\epsilon$  space-time dimensions

For each facet  $f \in F_{\Delta}^{N-1}$  a singularity is present in  $G$  if

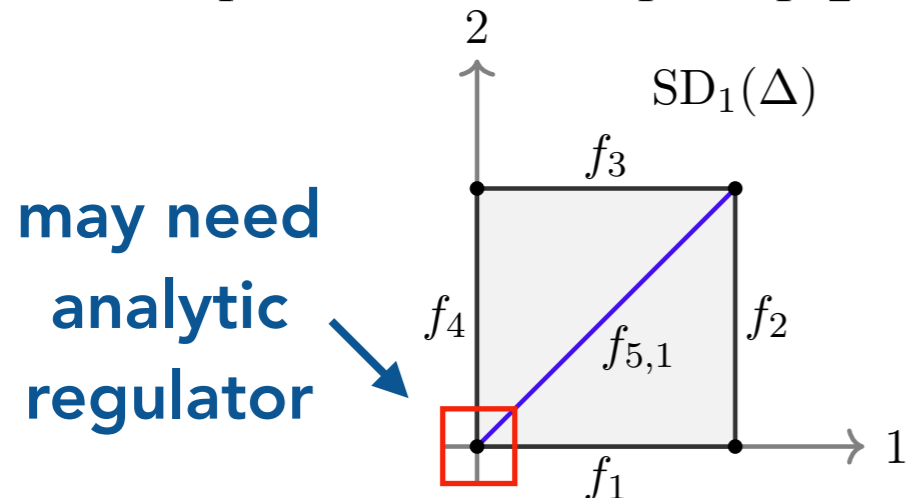
$$\langle \mathbf{v}_f, \nu \rangle + a_f \frac{D}{2} \leq 0 \quad \text{e.g: Schlenk 16}$$

EBR will effectively subdivide the Newton polytope (by selecting only certain vertices for each expansion), this will introduce new **internal facets**

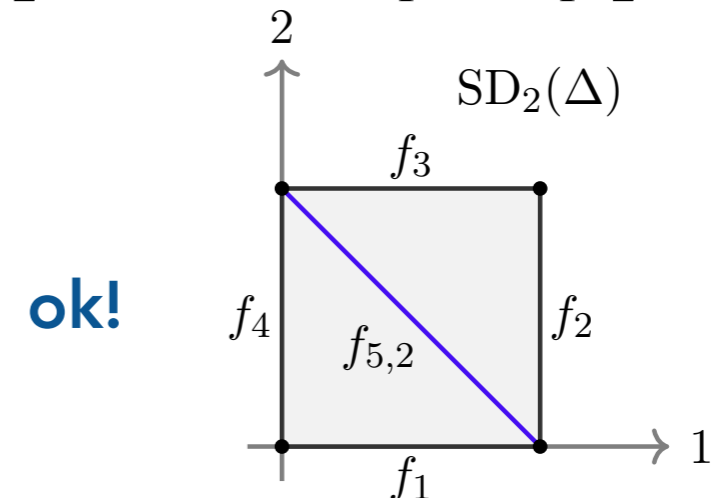
If these facets define a hyperplane that goes through  $\mathbf{0}$  (i.e.  $a_f = 0$ ) we can encounter spurious singularities, can introduce analytic regulators  $\nu \rightarrow \nu + \delta\nu_{\delta}$  to regulate them

**Examples:**

$$P_1(x, t) = 1 + tx_1 + x_1x_2 + tx_2$$



$$P_2(x, t) = t + x_1 + tx_1x_2 + x_2$$



# Geometric Method: Negative Coefficients

**Issue 2:** What happens if we have negative coefficients  $c_i < 0$ ? ← **not handled by pySecDec (yet!)**

Consider a 1-loop massive bubble at threshold  $y = m^2 - q^2/4 \rightarrow 0$

$$\mathcal{F} = q^2/4(x_1 - x_2)^2 + y(x_1 + x_2)^2$$

Can split integral into two subdomains  $x_1 \leq x_2$  and  $x_2 \leq x_1$  then remap

$$\begin{aligned} x_1 &= x'_1/2 \\ x_2 &= x'_2 + x'_1/2 \end{aligned} : \quad \mathcal{F} \rightarrow \frac{q^2}{4}x'^2_2 + y(x'_1 + x'_2)^2 \quad (\text{for first domain})$$

Various tools attempt to find such re-mappings:

**FIESTA** [Jantzen, A. Smirnov, V. Smirnov 12](#)

Check all pairs of variables  $(x_1, x_2)$  which are part of monomials of opposite sign

For each pair, try to build linear combination  $x'_1$  s.t negative monomial vanishes

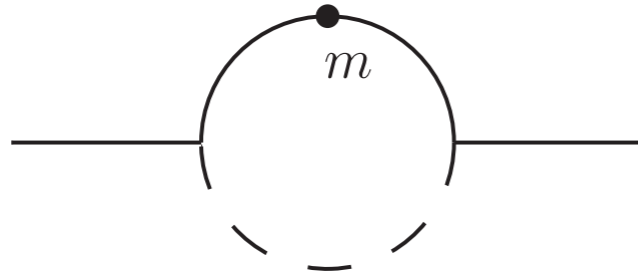
Repeat until all negative monomials vanish **or** warn user

**ASPIRE** [Ananthanarayan, Pal, Ramanan, Sarkar 18; B. Ananthanarayan, Das, Sarkar 20](#)

Consider Gröbner basis of  $\{\mathcal{F}, \partial\mathcal{F}/x_1, \partial\mathcal{F}/x_2, \dots\}$  (i.e.  $\mathcal{F}$  and Landau equations)

Eliminate negative monomials with linear transformations  $x_1 \rightarrow ax'_1, x_2 \rightarrow x'_2 + ax'_1$

# pySecDec: EBR Bubble Example



$$G = \mu^{2\epsilon} \int \frac{d^d k}{i\pi^{d/2}} \frac{1}{(k+p)^2 (k^2 - m^2)^2}$$

## Step 1: Define Integral & Expand

```
from pySecDec import LoopIntegralFromPropagators, loop_regions, sum_package

# guard the code to allow multiprocessing inside pySecDec
if __name__ == "__main__":

    # define the loop integral for the case where we expand in msq
    li_m = LoopIntegralFromPropagators(
        propagators = ("(k+p)**2", "k**2-msq"),
        loop_momenta = ["k"],
        powerlist = [1, 2],
        regulators = ["eps"],
        replacement_rules = [("p*p", "psq")])

    # find the regions and expand the integrals using expansion
    # by regions
    sum_terms = loop_regions(
        name = "bubble1L_dotted_m",
        loop_integral = li_m,
        smallness_parameter = "msq",
        expansion_by_regions_order = 1)

    # generate code that will calculate the sum of all regions
    # and the requested orders in the smallness parameter
    sum_package("bubble1L_dotted_m", sum_terms,
        regulators = li_m.regulators,
        requested_orders = [0],
        real_parameters = ["psq", "msq"],
        complex_parameters = [])
```

Define dotted  
1-loop bubble

Find regions  
assuming  
small msq/psq

Generate  
code

## Output region vectors:

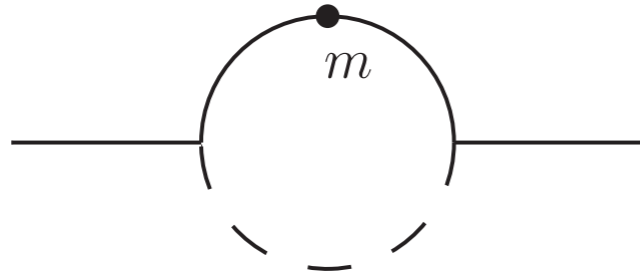
$$\mathbf{v}_1 = (0, -1, 1)$$

$$\mathbf{v}_2 = (0, 0, 1)$$

Also outputs a C++ code which can numerically compute the sum of the expanded integrals



# pySecDec: EBR Example



$$G = \mu^{2\epsilon} \int \frac{d^d k}{i\pi^{d/2}} \frac{1}{(k+p)^2 (k^2 - m^2)^2}$$

## Step 2: Integrate

```
from pySecDec.integral_interface import IntegralLibrary, series_to_sympy
import sympy as sp

if __name__ == "__main__":

    psq, msq = 4, 0.002
    name = "bubble1L_dotted_m"
    real_parameters = [psq, msq]

    # load the library
    intlib = IntegralLibrary(f"{name}/{name}_pylink.so")
    intlib.use_Qmc(transform="korobov3")

    # integrate
    integral_without_prefactor, prefactor, integral_with_prefactor = \
        intlib(real_parameters)

    # convert the result to sympy expressions
    result, error = \
        map(sp.sympify, series_to_sympy(integral_with_prefactor))

    # access and print individual terms of the expansion
    print("Numerical Result")
    for power in [-2, -1, 0]:
        val = complex(result.coeff("eps", power))
        err = complex(error.coeff("eps", power))
        print(f"eps^{power:<2} {val: .5f} +/- {err:.5e}")
```

## Step 3: Generate, Compile, Run

```
$ python3 generate_bubble1L_dotted_m_ebr.py
$ export CXX=nvcc
$ export SECDEC_WITH_CUDA_FLAGS="-gencode arch=compute_70,code=sm_70"
$ make -C bubble1L_dotted_m -j 8
$ time python3 integrate_bubble1L_dotted_m_ebr.py
> Numerical Result:
eps^-2  0.00000+0.00000j +/- 0.00000e+00+0.00000e+00j
eps^-1  0.00000+0.00000j +/- 1.87110e-17+0.00000e+00j
eps^0   1.90010-0.78540j +/- 8.70722e-17+1.03484e-16j
...

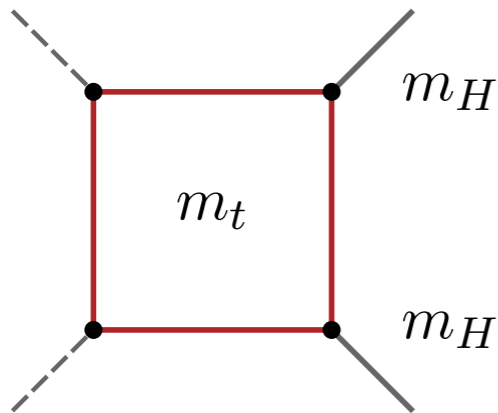
real    0m1.062s
user    0m2.175s
sys     0m0.270s
```

We have determined the Feynman parametrisation of our integral, applied expansion by regions and generated integrals which we then numerically computed

Of course, this works also for higher loop integrals...

# pySecDec: EBR Box Example

**Example:** 1-loop massive box expanded for small  $m_t^2 \ll s, |t|$



Requires the use of analytic regulators

Can regulate spurious singularities by adjusting propagators powers

$$G_4 = \mu^{2\epsilon} \int_{-\infty}^{\infty} \frac{d^D k}{i\pi^{D/2}} \frac{1}{[k^2 - m_t^2]^{\delta_1} [(k + p_1)^2 - m_t^2]^{\delta_2} [(k + p_1 + p_2)^2 - m_t^2]^{\delta_3} [(k - p_4)^2 - m_t^2]^{\delta_4}}$$

Can keep  $\delta_1, \dots, \delta_4$  symbolic or  $\delta_1 = 1 + n_1/2, \delta_2 = 1 + n_1/3, \dots$  and take  $n_1 \rightarrow 0^+$

**Output region vectors:**

$$\mathbf{v}_1 = (0, 0, 0, 0, 1)$$

$$\mathbf{v}_2 = (-1, -1, 0, 0, 1)$$

$$\mathbf{v}_3 = (0, 0, -1, -1, 1)$$

$$\mathbf{v}_4 = (-1, 0, 0, -1, 1)$$

$$\mathbf{v}_5 = (0, -1, -1, 0, 1)$$

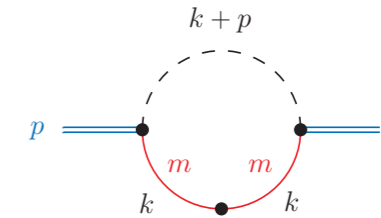
**Result:**  $s = 4.0, t = -2.82843, m_t^2 = 0.1, m_h^2 = 0$

$$I = -1.30718 \pm 2.7 \cdot 10^{-6} + (1.85618 \pm 3.0 \cdot 10^{-6}) i$$

$$+ \mathcal{O} \left( \epsilon, n_1, \frac{m_t^2}{s}, \frac{m_t^2}{t} \right)$$

Transform the expression for the full integral:

$$\begin{aligned}
 F &= \int_{k \in D_h} \mathrm{D}k I + \int_{k \in D_s} \mathrm{D}k I = \sum_i \int_{k \in D_h} \mathrm{D}k T_i^{(h)} I + \sum_j \int_{k \in D_s} \mathrm{D}k T_j^{(s)} I \\
 &= \sum_i \left( \int_{k \in \mathbb{R}^d} \mathrm{D}k T_i^{(h)} I - \sum_j \int_{k \in D_s} \mathrm{D}k T_j^{(s)} T_i^{(h)} I \right) + \sum_j \left( \int_{k \in \mathbb{R}^d} \mathrm{D}k T_j^{(s)} I - \sum_i \int_{k \in D_h} \mathrm{D}k T_i^{(h)} T_j^{(s)} I \right)
 \end{aligned}$$



The **expansions commute**:  $T_i^{(h)} T_j^{(s)} I = T_j^{(s)} T_i^{(h)} I \equiv T_{i,j}^{(h,s)} I$

$$\Rightarrow \text{Identity: } F = \underbrace{\sum_i \int \mathrm{D}k T_i^{(h)} I}_{F^{(h)}} + \underbrace{\sum_j \int \mathrm{D}k T_j^{(s)} I}_{F^{(s)}} - \underbrace{\sum_{i,j} \int \mathrm{D}k T_{i,j}^{(h,s)} I}_{F^{(h,s)}}$$

All terms are integrated over the **whole integration domain**  $\mathbb{R}^d$  as prescribed for the expansion by regions  $\Rightarrow$  location of **boundary**  $\Lambda$  between  $D_h, D_s$  is **irrelevant**.

## The general formalism (details)

Identities as in the examples are **generally valid**, under some conditions.

### Consider

- a (multiple) integral  $F = \int_D k I$  over the domain  $D$  (e.g.  $D = \mathbb{R}^d$ ),
- a set of  $N$  regions  $R = \{x_1, \dots, x_N\}$ ,
- for each region  $x \in R$  an expansion  $T^{(x)} = \sum_j T_j^{(x)}$  which converges absolutely in the domain  $D_x \subset D$ .

### Conditions

- $\bigcup_{x \in R} D_x = D$       $[D_x \cap D_{x'} = \emptyset \ \forall x \neq x']$ .
- Some of the **expansions commute** with each other.  
Let  $R_c = \{x_1, \dots, x_{N_c}\}$  and  $R_{nc} = \{x_{N_c+1}, \dots, x_N\}$  with  $1 \leq N_c \leq N$ .  
Then:  $T^{(x)} T^{(x')} = T^{(x')} T^{(x)} \equiv T^{(x, x')} \ \forall x \in R_c, x' \in R$ .
- Every pair of non-commuting expansions is invariant under some expansion from  $R_c$ :  
 $\forall x'_1, x'_2 \in R_{nc}, x'_1 \neq x'_2, \exists x \in R_c : T^{(x)} T^{(x'_2)} T^{(x'_1)} = T^{(x'_2)} T^{(x'_1)}$ .
- $\exists$  **regularization** for singularities, e.g. dimensional (+ analytic) regularization.  
 $\hookrightarrow$  All expanded integrals and series expansions in the formalism are well-defined.

## The general formalism (2)

Under these conditions, the following **identity** holds:  $[F^{(x,\dots)} \equiv \sum_{j,\dots} \int Dk T_{j,\dots}^{(x,\dots)} I]$

$$F = \sum_{x \in R} F^{(x)} - \sum_{\{x'_1, x'_2\} \subset R}^{\langle R_c + 1 \rangle} F^{(x'_1, x'_2)} + \dots - (-1)^n \sum_{\{x'_1, \dots, x'_n\} \subset R}^{\langle R_c + 1 \rangle} F^{(x'_1, \dots, x'_n)} + \dots + (-1)^{N_c} \sum_{x' \in R_{nc}} F^{(x', x_1, \dots, x_{N_c})}$$

where the sums run over subsets  $\{x'_1, \dots\}$  containing at most one region from  $R_{nc}$ .

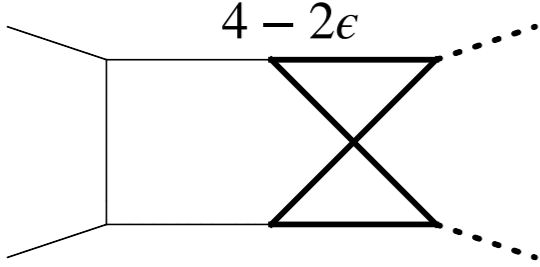
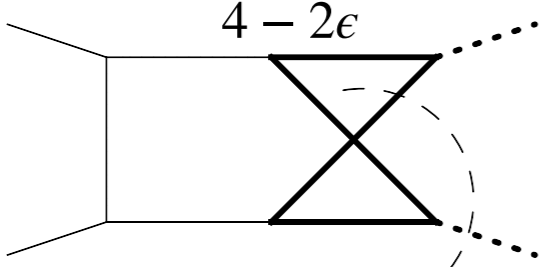
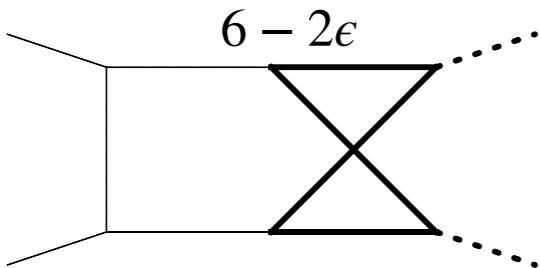
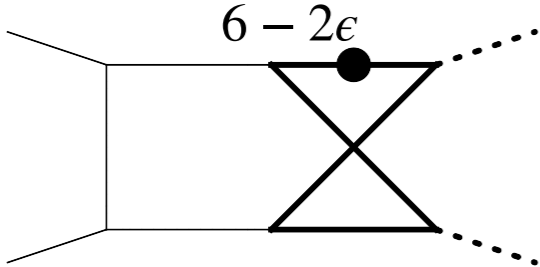
### Comments

- This identity is **exact** when the expansions are summed to all orders. ✓  
Leading-order approximation for  $F \rightsquigarrow$  dropping higher-order terms.
- It is **independent of the regularization** (dim. reg., analytic reg., cut-off, infinitesimal masses/off-shellness, ...) as long as all individual terms are well-defined.
- Usually regions & regularization are chosen such that **multiple expansions**  $F^{(x'_1, \dots, x'_n)}$  ( $n \geq 2$ ) are **scaleless** and vanish.  
[✓ if each  $F_0^{(x)}$  is a *homogeneous* function of the expansion parameter with *unique scaling*.]
- If  $\exists F^{(x'_1, x'_2, \dots)} \neq 0 \rightsquigarrow$  relevant **overlap contributions** ( $\rightarrow$  “zero-bin subtractions”).  
They appear e.g. when avoiding analytic regularization in SCET. e.g. Manohar, Stewart '06;  
Chiu, Fuhrer, Hoang, Kelley, Manohar '09; ...

# Numerical Integration

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# Finite Integrals (example from $gg \rightarrow ZZ$ )

	Finite	$\epsilon$ Order	Rel Err	Timing (s)
	No	0	$2 \cdot 10^{-3}$	45
	No	0	$4 \cdot 10^{-2}$	63
	Yes	1	$8 \cdot 10^{-6}$	60
	Yes	1	$8 \cdot 10^{-4}$	55
Linear combination (numerator insertion)	Yes	1	$1 \cdot 10^{-4}$	18

Figures & Timings: Bakul Agarwal

pySecDec + QMC  
Nvidia Tesla V100

# Numerical Integration

$$I[f] \equiv \int_{[0,1]^d} d\mathbf{x} f(\mathbf{x}) \approx Q[f] = \frac{1}{N} \sum_{i=1}^N w_i f(\mathbf{x}_i)$$

Goal: select points to minimise integration error

$$\varepsilon \equiv |I[f] - Q[f]|$$

## Monte Carlo:

Randomly select sampling points

$$\varepsilon \approx \text{Var}[f]/\sqrt{N}, \quad \varepsilon \sim \mathcal{O}(N^{-1/2})$$

Improves slowly with  $N$

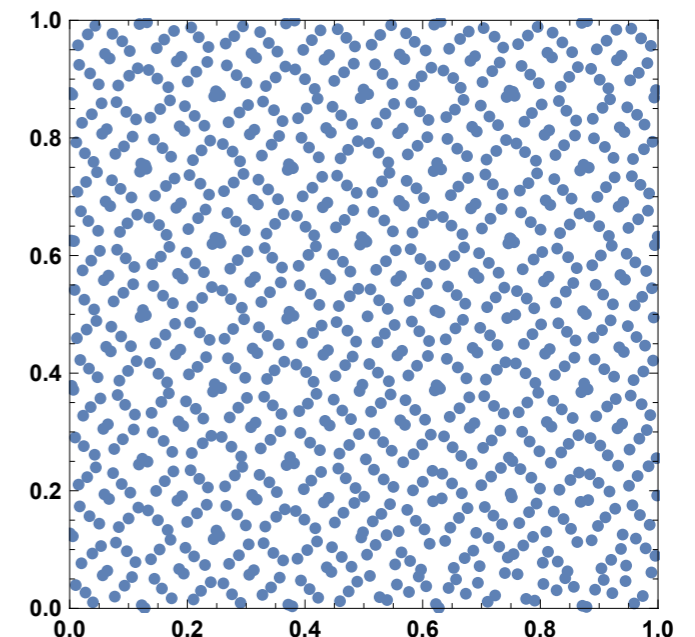
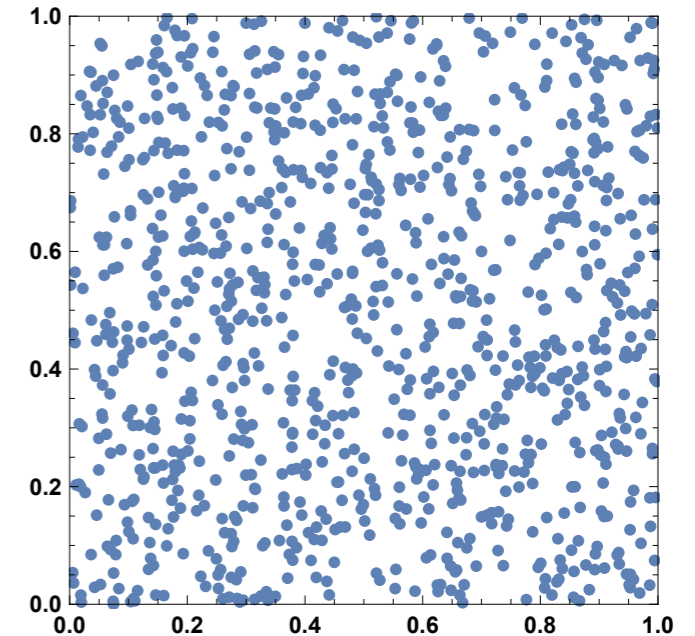
## Quasi-Monte Carlo

Select points with low discrepancy  $D_N$

$$\varepsilon \leq D_N \cdot \text{Var}[f], \quad \varepsilon \sim \mathcal{O}(\log^d(N)/N)$$

Poor performance for large  $d$

Both methods implemented in Cuba [Hahn 04](#); [Hahn14](#)





# Quasi-Monte Carlo (Rank 1 Lattices)

## Quasi-Monte Carlo (QMC) in a Weighted Function Space

First applications to loop integrals, see:

Li, Wang, Yan, Zhao 15; de Doncker, Almulihi, Yuasa 17, 18; de Doncker, Almulihi 17;

$$\varepsilon \leq e_\gamma \cdot \|f\|_\gamma, \quad \varepsilon \sim \mathcal{O}(N^{-1}) \text{ or better}$$

Kato, de Doncker, Ishikawa, Yuasa 18

$$I[f] \approx \bar{Q}_{n,m}[f] \equiv \frac{1}{m} \sum_{k=0}^{m-1} Q_n^{(k)}[f], \quad Q_n^{(k)}[f] \equiv \frac{1}{n} \sum_{i=0}^{n-1} f \left( \left\{ \frac{i\mathbf{z}}{n} + \Delta_k \right\} \right)$$

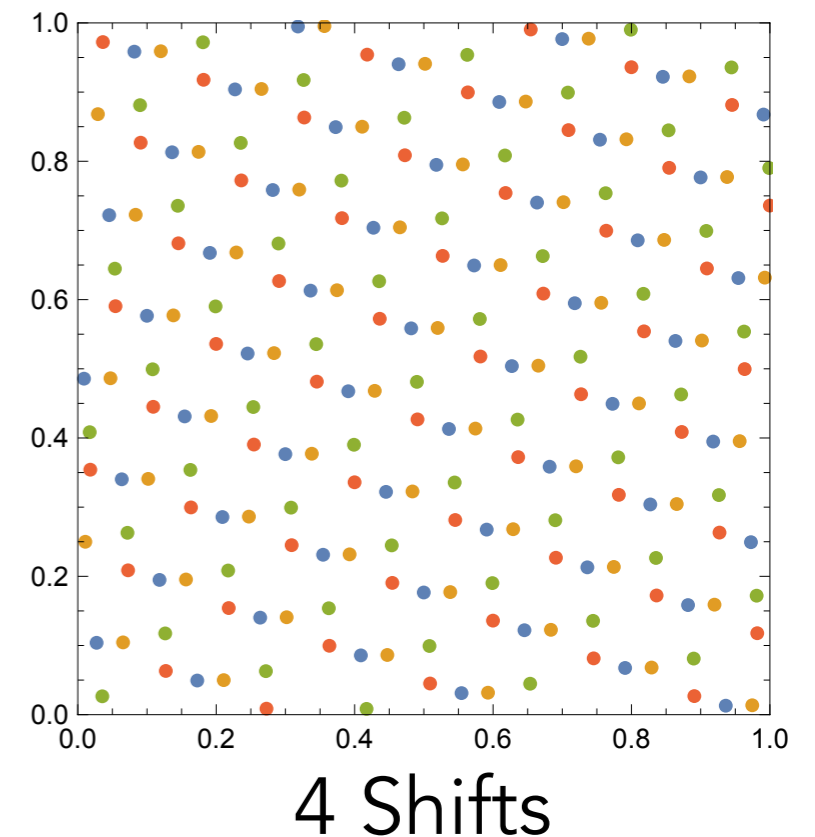
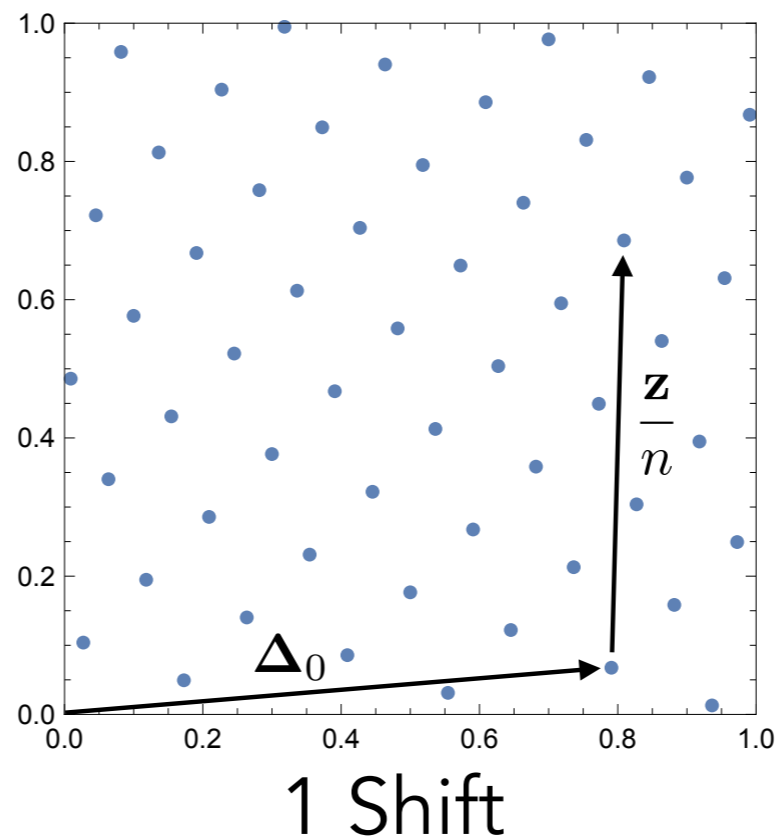
$\mathbf{z}$  - Generating vec.

$\Delta_k$  - Random shift vec.

$\{ \}$  - Fractional part

$n$  - # Lattice points

$m$  - # Random shifts



Unbiased error estimate computed using (10-50) random shifts

# Weighted Function Spaces

Assign weights  $\gamma_{\mathbf{u}}$  to each subset of dimensions  $\mathbf{u} \subseteq \{1, \dots, d\}$  Review: Dick, Kuo, Sloan 13

## Sobolev Space

Functions with square integrable first derivatives

Norm 
$$\|f\|_{\gamma}^2 = \sum_{\mathbf{u} \subseteq \{1, \dots, d\}} \frac{1}{\gamma_{\mathbf{u}}} \int_{[0,1]^{|\mathbf{u}|}} \left( \int_{[0,1]^{d-|\mathbf{u}|}} \frac{\partial^{|\mathbf{u}|} f(\mathbf{x})}{\partial \mathbf{x}_{\mathbf{u}}} d\mathbf{x}_{-\mathbf{u}} \right)^2 d\mathbf{x}_{\mathbf{u}}$$

Worst-case error 
$$e_{\gamma}^2 \leq \left( \frac{1}{\psi(n)} \sum_{\emptyset \neq \mathbf{u} \subseteq \{1, \dots, d\}} \gamma_{\mathbf{u}}^{\lambda} \left( \frac{2\zeta(2\lambda)}{(2\pi^2)^{\lambda}} \right)^{|\mathbf{u}|} \right)^{\frac{1}{\lambda}}$$
  
 $\forall \lambda \in (1/2, 1]$

$\varepsilon \sim \mathcal{O}(n^{-1})$

## Korobov Space

Periodic functions which are  $\alpha$  times differentiable in each variable

Norm 
$$\|f\|_{\gamma}^2 = \sum_{\mathbf{h} \in \mathbb{Z}^d} \frac{\prod_{j \in \mathbf{u}(\mathbf{h})} |h_j|^{2\alpha}}{\gamma_{\mathbf{u}(\mathbf{h})}} |\hat{f}(\mathbf{h})|^2$$
  
↑  
Fourier Coefficient

Worst-case error 
$$e_{\gamma}^2 \leq \left( \frac{1}{\psi(n)} \sum_{\emptyset \neq \mathbf{u} \subseteq \{1, \dots, d\}} \gamma_{\mathbf{u}}^{\lambda} (2\zeta(2\alpha\lambda))^{|\mathbf{u}|} \right)^{\frac{1}{\lambda}}$$
  
 $\forall \lambda \in (1/(2\alpha), 1], \text{ smoothness } \alpha$

$\varepsilon \sim \mathcal{O}(n^{-\alpha})$

Generating vector  $\mathbf{z}$  precomputed for a **fixed** number of lattice points, chosen to minimise the worst-case error, we use component-by-component (CBC) construction Nuyens 07

In our public code, we distribute lattice rules generated using product weights:

$\gamma_{\mathbf{u}} = \prod_{i \in \mathbf{u}} \gamma_i, \gamma_i = 1/d$  produced for a Korobov space with  $\alpha = 2$

# Periodising Transforms

Lattice rules work especially well for continuous, smooth and periodic functions  
Functions can be periodized by a suitable change of variables:  $\mathbf{x} = \phi(\mathbf{u})$

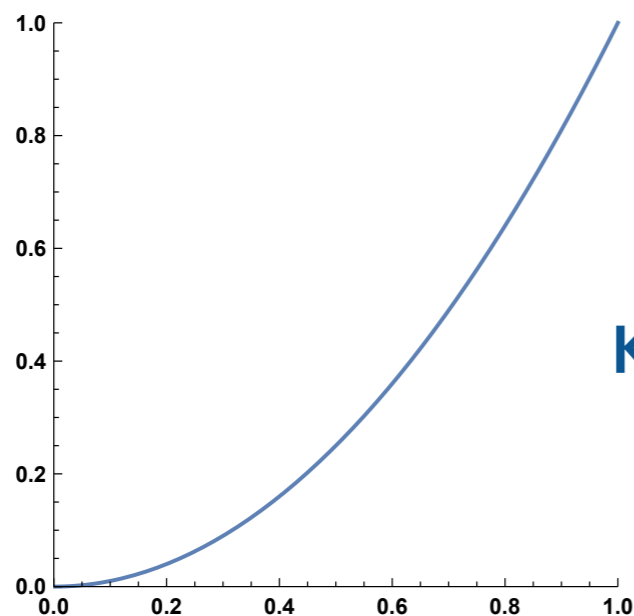
$$I[f] \equiv \int_{[0,1]^d} d\mathbf{x} f(\mathbf{x}) = \int_{[0,1]^d} d\mathbf{u} \omega_d(\mathbf{u}) f(\phi(\mathbf{u}))$$

$$\phi(\mathbf{u}) = (\phi(u_1), \dots, \phi(u_d)), \quad \omega_d(\mathbf{u}) = \prod_{j=1}^d \omega(u_j) \quad \text{and} \quad \omega(u) = \phi'(u)$$

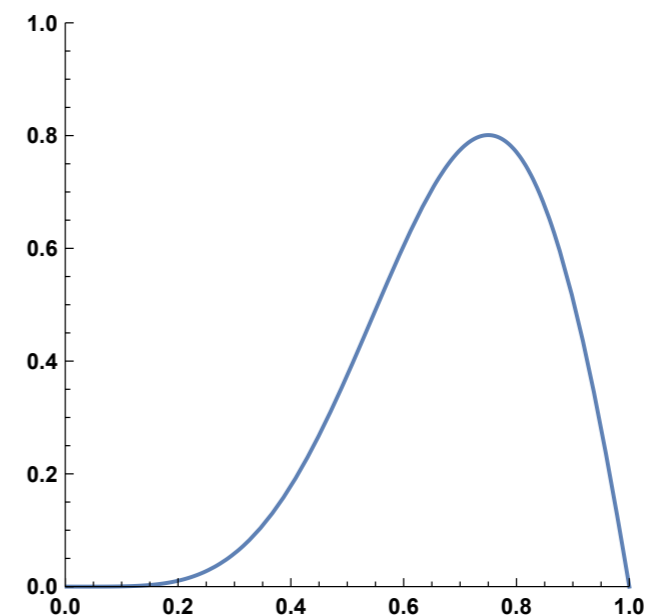
**Korobov transform:**  $\omega(u) = 6u(1-u)$ ,  $\phi(u) = 3u^2 - 2u^3$

**Sidi transform:**  $\omega(u) = \pi/2 \sin(\pi u)$ ,  $\phi(u) = 1/2(1 - \cos \pi t)$

**Baker transform:**  $\phi(u) = 1 - |2u - 1|$



**Korobov transform**

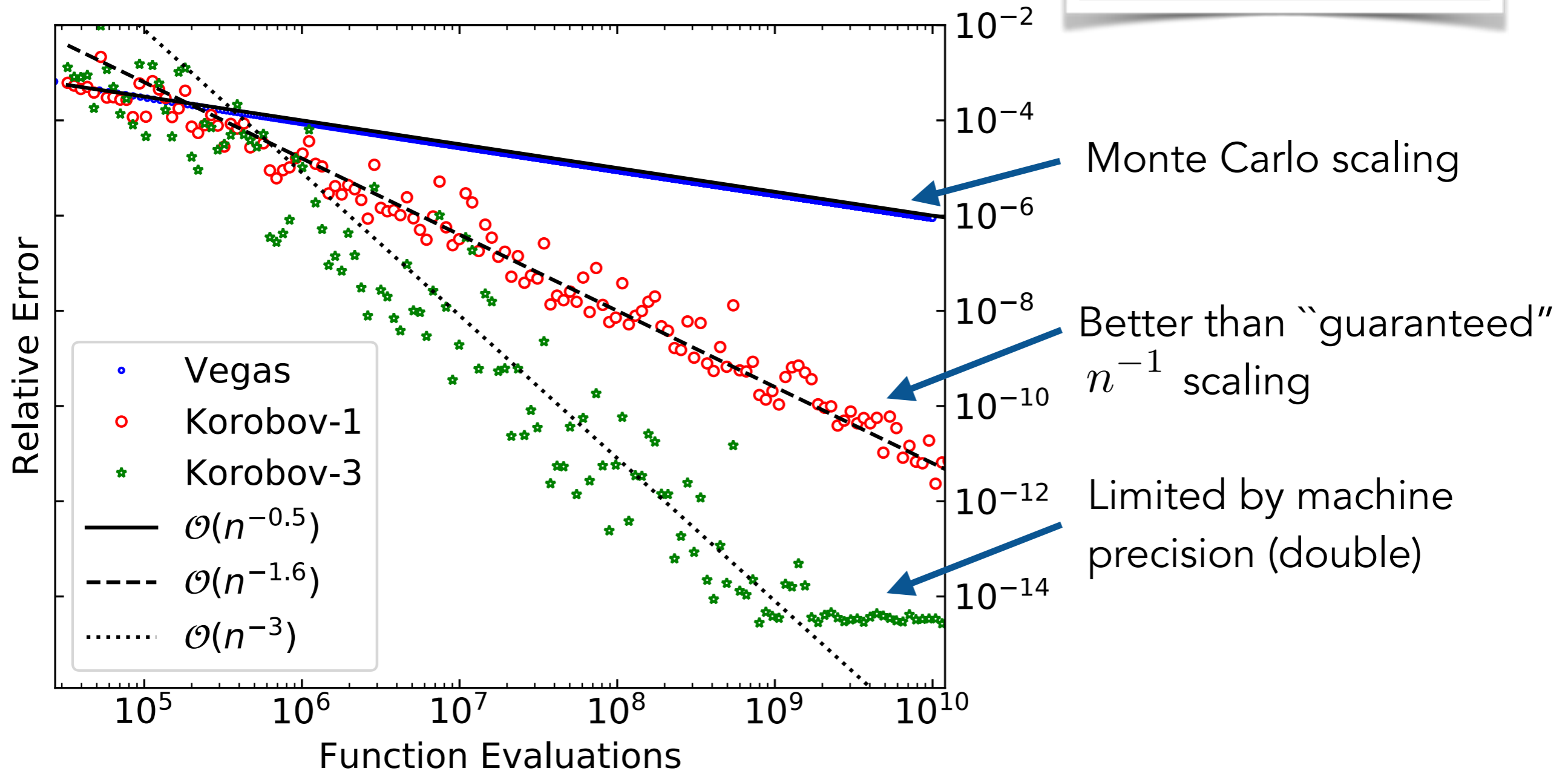
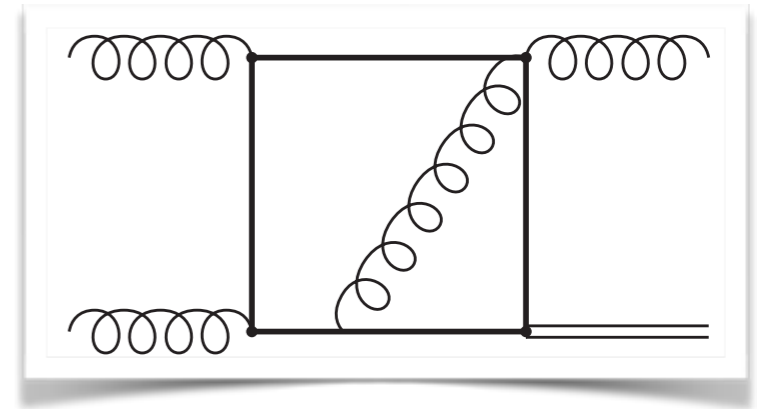


# Scaling

## Example:

Sector Decomposed HJ Integral

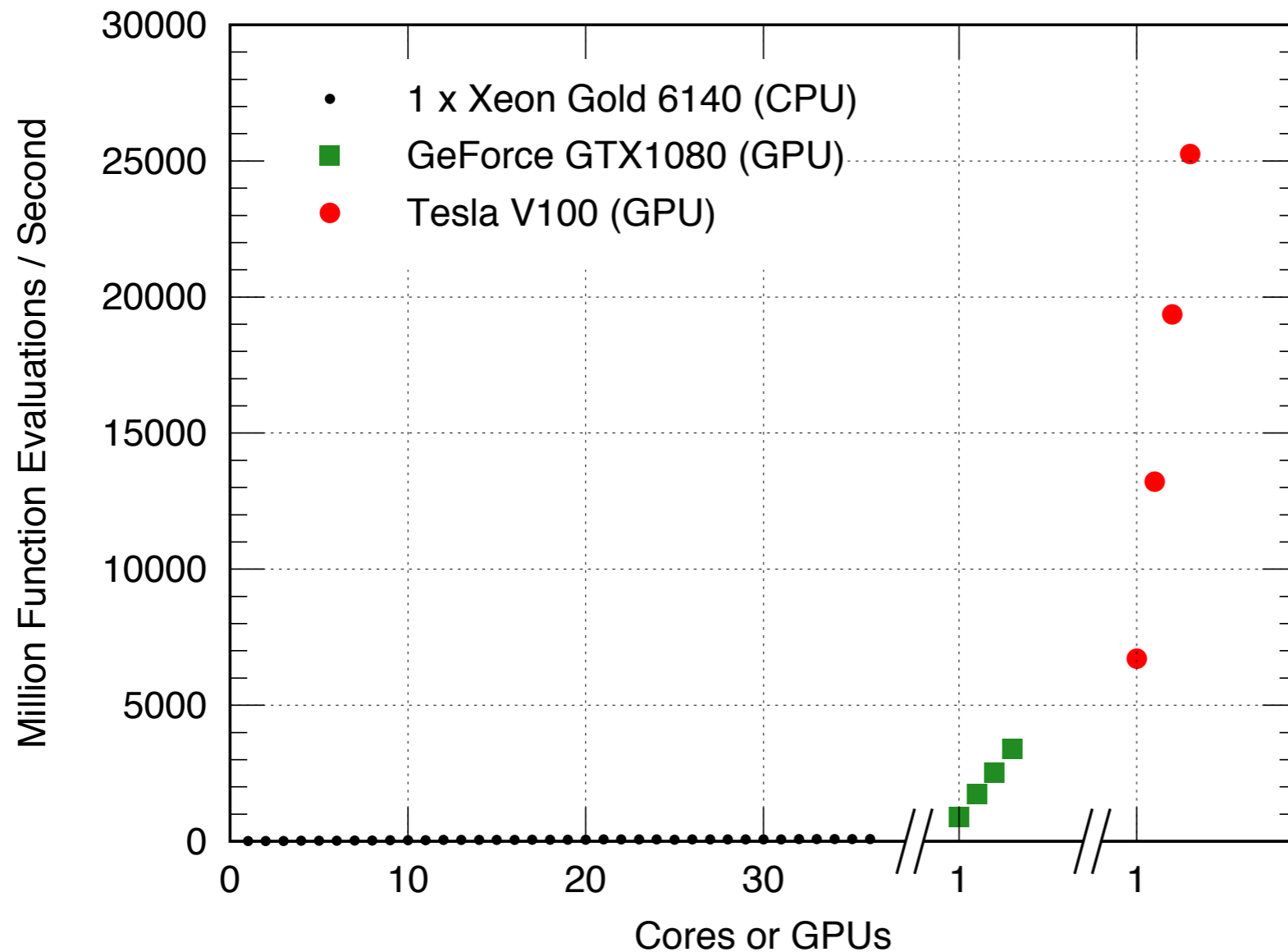
(Note: example stolen from previous calculation)



# qmc: Performance

Accuracy limited by number of function evaluations

Can accelerate this using Graphics Processing Units (GPUs)



Device	M Func. Evals/s	Speedup
Xeon 6140	80.6	-
GTX1080	897	11x
Tesla V100	6710	83x

**Note:** Performance gain highly dependent on integrand & hardware!  
Still room for further optimisations (both for CPU and GPU)