Numerical multi-loop calculations with pySecDec

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Numerical results for two-loop amplitudes

Differential equations

$pp \to t\bar{t}$ Czakon, Fiedler, Heymes, Mitov ('13,'16,'17)

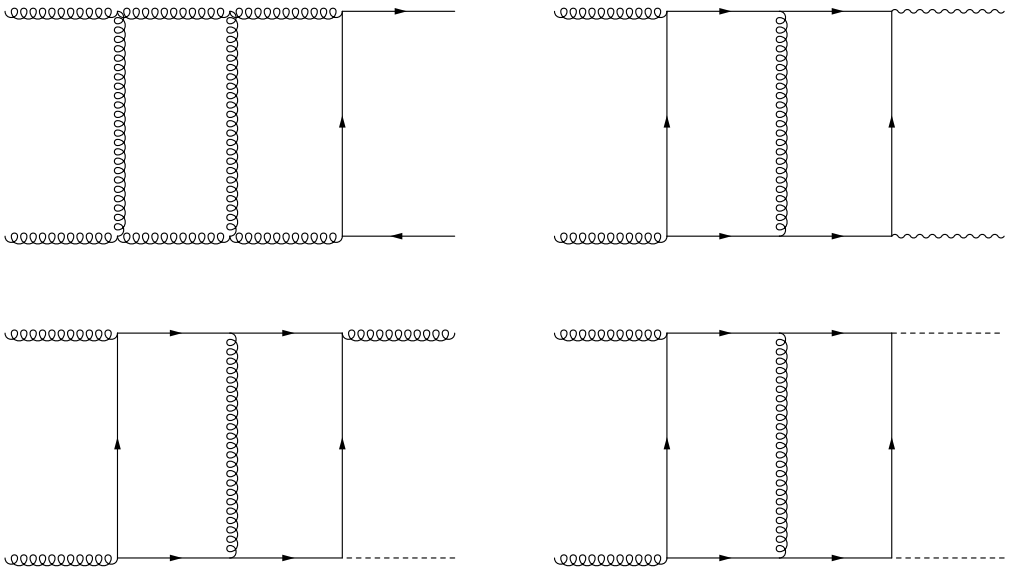
$gg \to \gamma\gamma$ Mandal, Maltoni, Zhao (2019)

Sector decomposition

$pp \to HH$ Borowka, Greiner, Heinrich, Jones, Kerner, JS, Schubert, Zirke (2016)

$pp \to HJ$ Jones, Kerner, Luisoni (2018)

$pp \to HH$ (partial EW) Borowka, Duhr, Maltoni, Pagani, Shivaji, Zhao (2019)



Direct numerical integration

$pp \to HH$ Baglio, Campanario, Glaus, Mühlleitner, Spira, Streicher (2018)

Numerical calculation of Feynman integrals using sector decomposition

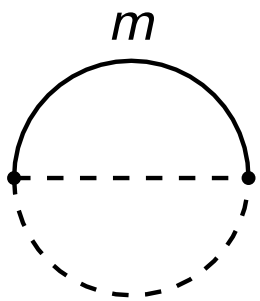
Hepp (1966); Denner, Roth (1996); Binoth, Heinrich (2000)

$$\int \frac{\prod_{l=1}^{L} \mathrm{d}^D k_l}{D_1^{\nu_1} \dots D_N^{\nu_N}} \sim \int_0^\infty \frac{\mathrm{d}\mathbf{x}}{\mathbf{x}} \mathbf{x}^\nu \, \delta(1-x_N) \frac{\mathcal{U}(\mathbf{x})^{N-(L+1)D/2}}{\mathcal{F}(\mathbf{x}, s_{ij})^{N-LD/2}} = \frac{c_{-2L}}{\epsilon^{2L}} + \frac{c_{-2L+1}}{\epsilon^{2L-1}} + \dots$$

- Decompose integration region into sectors with simple singularity structure
- Contour deformation for multi-scale integrals in physical region Soper (2000);Binoth, Guillet, Heinrich, Pilon, Schubert (2005); Nagy, Soper (2006); Borowka, Heinrich (2012)
- Subtract divergences and expand in the regularization parameter ϵ
- Integrate the finite coefficients (numerically)
- Applicable to loop integrals and more general parametric integrals

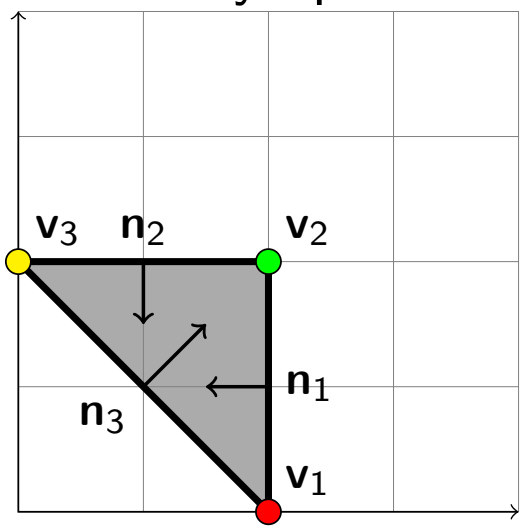
Geometric sector decomposition

Kaneko, Ueda (2010), Borowka, Heinrich, Jones, Kerner, JS, Zirke (2015)
other strategies: Binoth Heinrich (2000), Bogner, Weinzierl (2008), Smirnov, Tentyukov (2009)



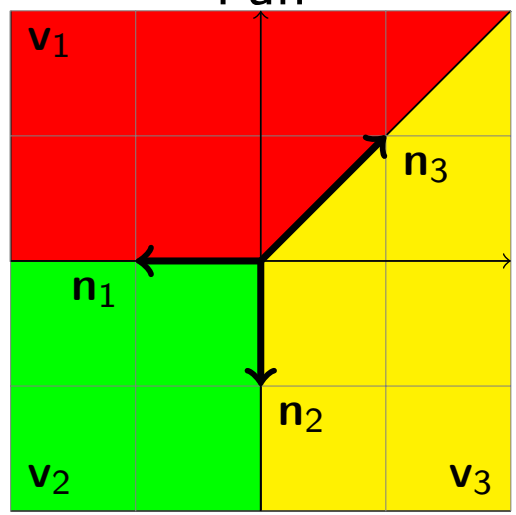
$$\sim \int_0^\infty \frac{\mathrm{d}x_1\,\mathrm{d}x_2}{x_1 x_2} x_1^{\nu_1} x_2^{\nu_2} \left(\underline{x_1^1 x_2^0} + \underline{x_1^1 x_2^1} + \underline{x_1^0 x_2^1}\right)^{-\frac{D}{2}}$$

Polytope



$$x_i = \prod_F y_F^{\langle \mathbf{n}_F, \hat{\mathbf{e}}_i \rangle}$$

Fan



$$= \int_0^1 \frac{\mathrm{d}y_1\,\mathrm{d}y_2\,\mathrm{d}y_3}{y_1 y_2 y_3} y_1^{-\nu_1+\frac{D}{2}}\, y_2^{-\nu_2+\frac{D}{2}}\, y_3^{\nu_1+\nu_2-\frac{D}{2}} (y_1+y_2+y_3)^{-\frac{D}{2}} \sum_{i=1}^{3} \delta(1-y_i)$$

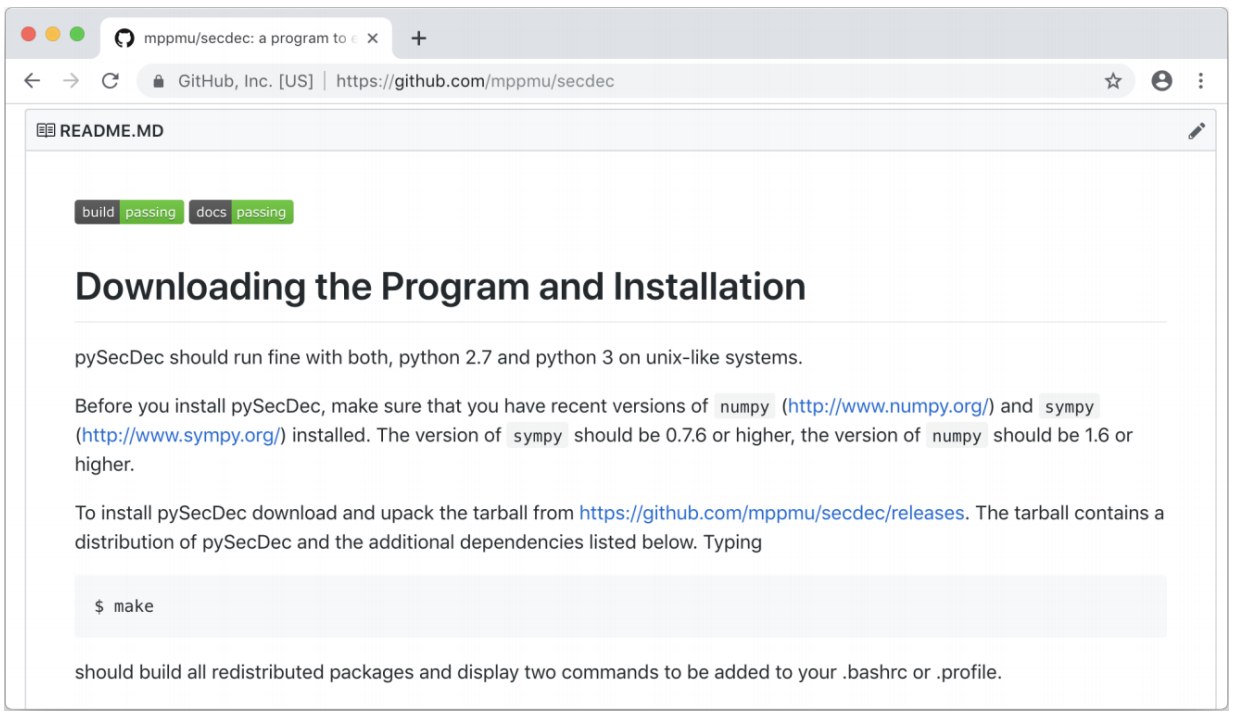
pySecDec

- Public implementation of the sector decomposition method (Python, C++, Form Vermaseren et al.) Borowka, Heinrich, Jahn, Jones, Kerner, JS, Zirke (2017)

  earlier versions: Carter, Heinrich (2010); Borowka, Heinrich (2012), Borowka, Heinrich, Jones, Kerner, JS, Zirke (2015)

Other public tools

- sector_decomposition + CSectors Bogner, Weinzierl (2007), Gluza, Kajda, Riemann, Yundin (2010)
- FIESTA Smirnov, Smirnov Tentyukov ('09, '11, '14, '15)



Numerical Integration

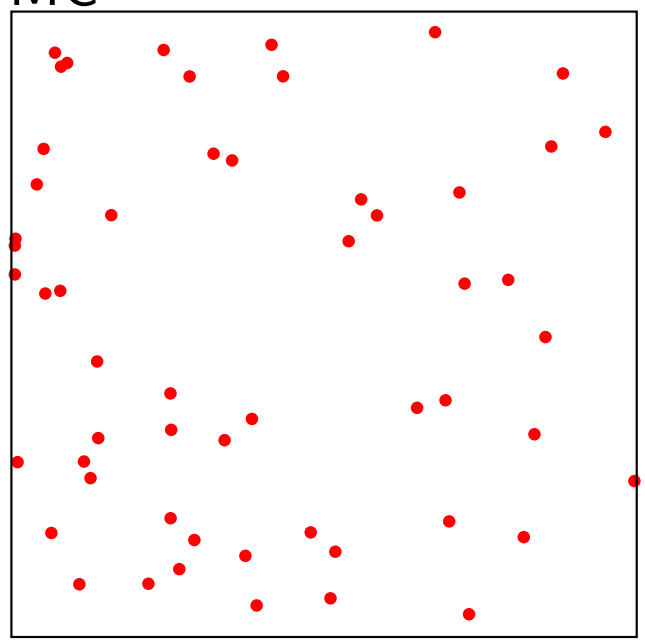
$$I_s(f) = \int_{[0,1]^s} \mathrm{d}\mathbf{x} f(\mathbf{x}) \to Q_{s,n}(f) = \frac{1}{n} \sum_{i=0}^{n-1} f(\mathbf{x}_i)$$

minimize error $\epsilon = |I_s(f) - Q_{s,n}(f)|$

Monte Carlo

- Integration points $\mathbf{x}_i$ randomly distributed
- $$\epsilon = \frac{\sigma(f)}{\sqrt{n}} \sim \mathcal{O}(n^{-1/2})$$
- Implemented in CUBA Hahn ('04, '14)

MC

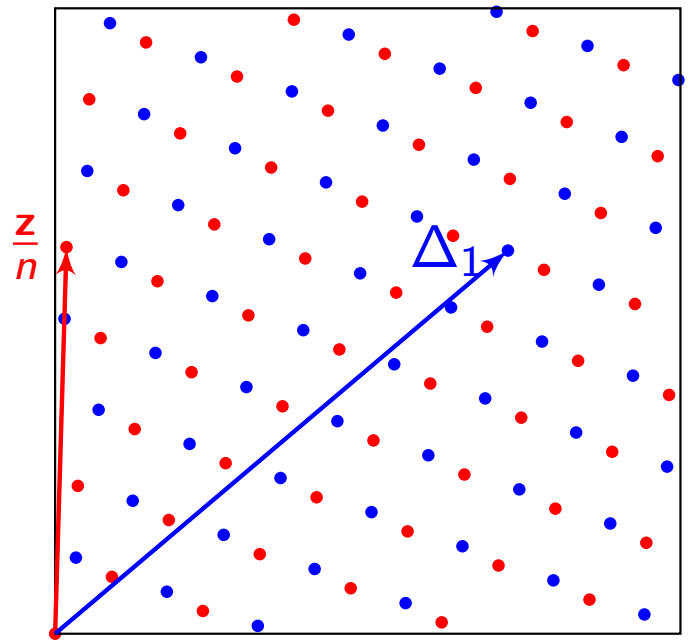


Quasi Monte Carlo

Dick, Kuo, Sloan (2013)

Rank-1 lattice rule: $\mathbf{x}_i = \left\{ \frac{i\mathbf{z}}{n} + \boldsymbol{\Delta}_k \right\}, \quad i = 0, \ldots, n-1$

- $\mathbf{z}$: generating vector
- $\{\ldots\}$: fractional part
- $\mathcal{O}(n^{-1})$ error scaling for certain classes of smooth, periodic functions
- First application to sector decomposition by Li, Wang, Yan, Zhao (2015)
- Shift lattice by random vectors $\boldsymbol{\Delta}_k$ to obtain error estimate



$$\bar{Q}_{s,n,m}(f) = \frac{1}{m} \sum_{k=0}^{m-1} Q_{s,n}^{(k)} \qquad Q_{s,n}^{(k)} = \frac{1}{n} \sum_{i=0}^{n-1} f\left(\left\{ \frac{i\mathbf{z}}{n} + \boldsymbol{\Delta}_k \right\} \right)$$

Periodization

Dick, Kuo, Sloan (2013)

Functions can be periodized by change of variables $\mathbf{x} = \psi(\mathbf{y})$:

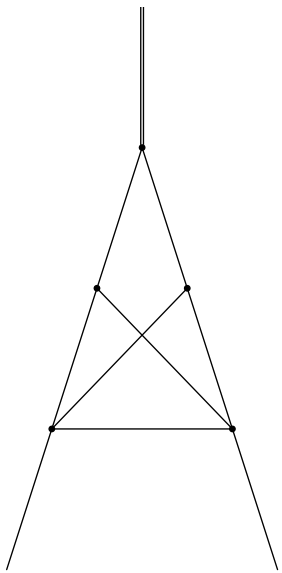
$$I_s(f) = \int_{[0,1]^s} \mathrm{d}\mathbf{x} f(\mathbf{x}) = \int_{[0,1]^s} \prod_{j=1}^{s} \mathrm{d}y_j \omega(y_j) f(\psi(\mathbf{y}))$$

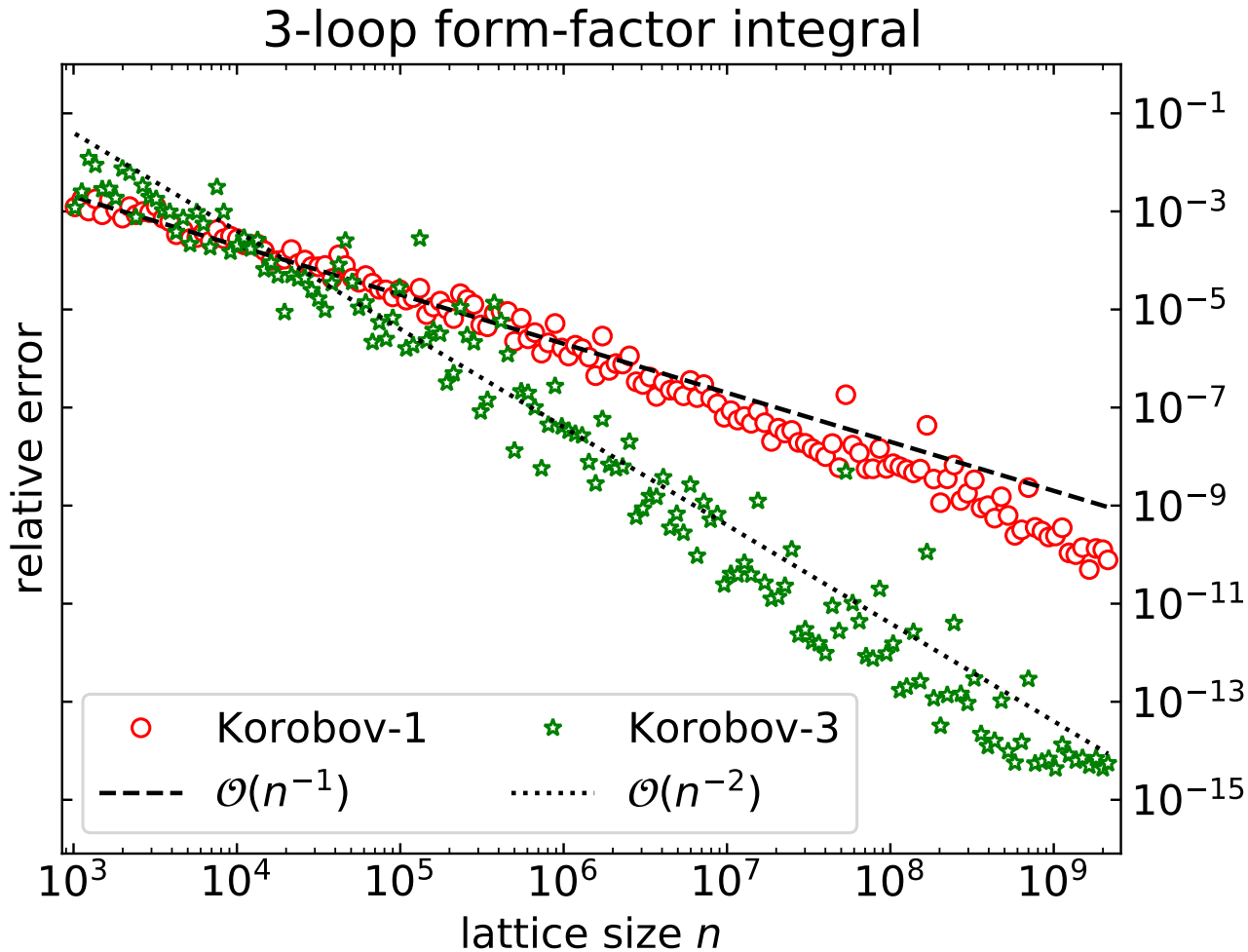
with $\psi'(y) = \omega(y)$

- Korobov: $\omega_{\alpha,\beta}(y) = (\alpha+\beta+1)\binom{\alpha+\beta}{\alpha} y^\alpha (1-y)^\beta$

  Korobov (1963), Laurie (1996), Kuo, Sloan, Wozniakowski (2007)
- Sidi: $\omega_\alpha(y) = \frac{\pi}{2^\alpha} \frac{\Gamma(\alpha+1)}{\Gamma((\alpha+1)/2)^2} sin(\pi y)^\alpha$ Sidi (1993)
- Baker: $\psi(y) = 1 - |1-2y|$ Hickernell (2002)

Scaling



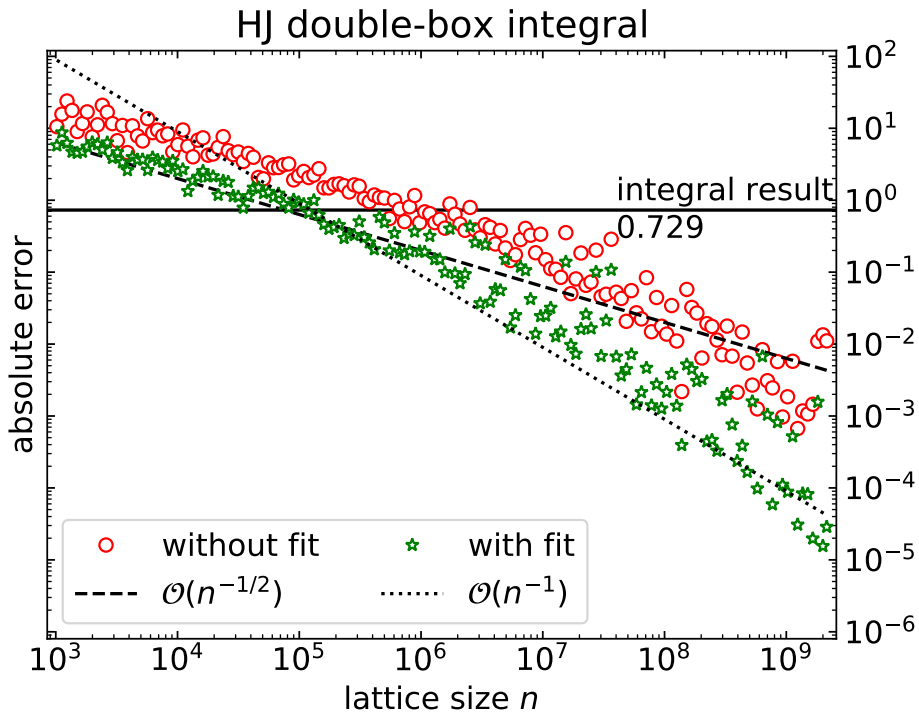

3-loop form-factor integral
relative error
lattice size n
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
10^{-15}
10^{3}
10^{4}
10^{5}
10^{6}
10^{7}
10^{8}
10^{9}
Korobov-1
Korobov-3
$\mathcal{O}(n^{-1})$
$\mathcal{O}(n^{-2})$

Variance reduction

Flatten integrand by change of variables $x = p(y)$ with $p'(y) \sim f(p(y))^{-1}$

$$\int_0^1 \mathrm{d}x f(x) = \int_0^1 \mathrm{d}y p'(y) f(p(y))$$

- Smooth function ansatz for $p(y)$ to preserve smoothness of integrand
- Free parameters fitted to inverse of cumulative distribution function



$$p(x) = a_2 \cdot x \frac{a_0 - 1}{a_0 - x} + a_3 \cdot x \frac{a_1 - 1}{a_1 - x} + a_4 \cdot x + a_5 \cdot x^2 + \left(1 - \sum_{i=2}^{5} a_i\right) \cdot x^3$$

QMC implementation

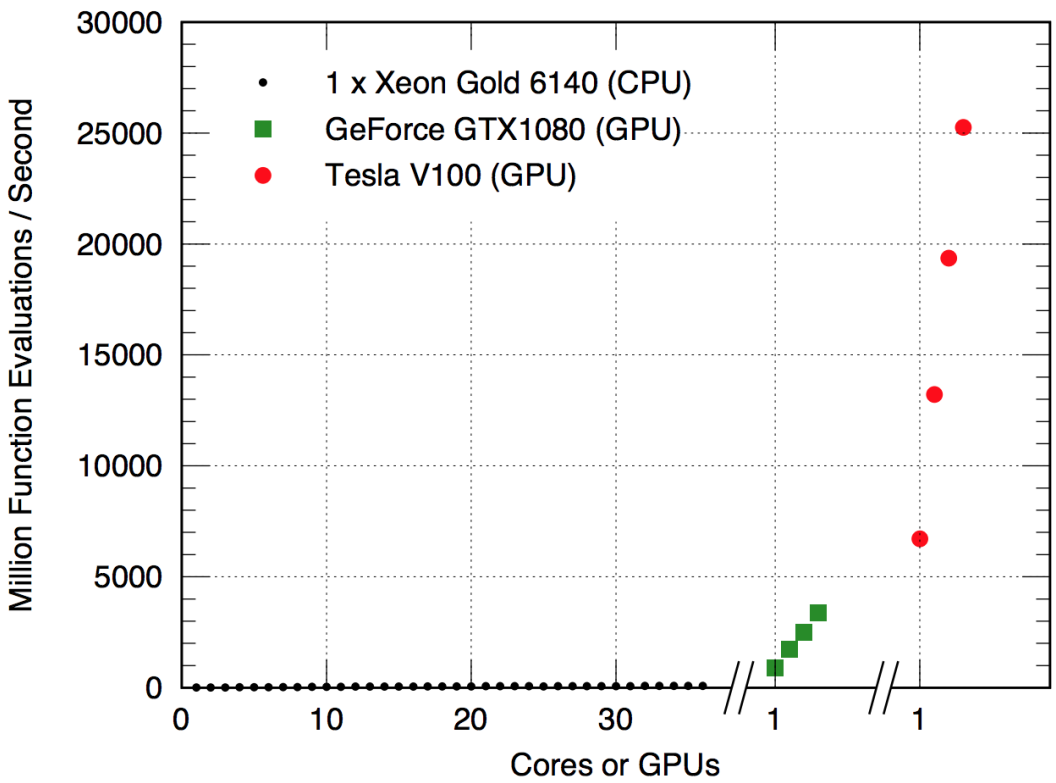
Public implementation of Quasi Monte Carlo integration Borowka, Heinrich, Jahn, Jones, Kerner, JS (2018)

github.com/mppmu/qmc

- Single header C++11 library using CUDA
- Parallelization over multiple GPUs and CPUs on a single machine

Device	M Func evals/s
Xeon 6140	80.6
GTX1080	897
V100	6710

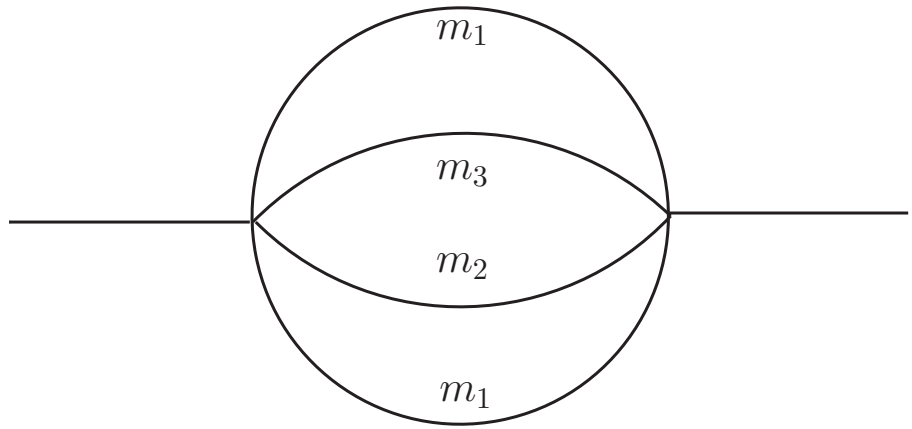
performance hugely dependent on integrand



Study and figure by Stephen Jones

Hyperelliptic integrals: 3 mass banana graph

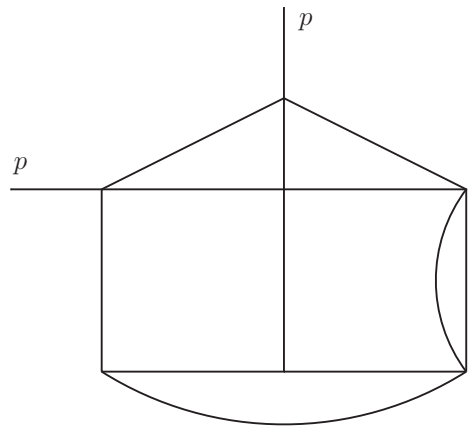
- New class of analytic functions
- $\rightarrow$ talk by L. Tancredi
- Unproblematic for numerical calculation
- $s = 20$, $m_1^2 = 1$, $m_2^2 = 1.3$, $m_3^2 = 0.7$
- `minn=1000000`, `transform='korobov2'`



$$
\begin{aligned}
I = &\left(1.97000000000000264 \pm 9.85 \cdot 10^{-15} + \mathrm{i}\left(1.84 \cdot 10^{-15} \pm 1.16 \cdot 10^{-15}\right)\right) \cdot \epsilon^{-3} \\
&+ \left(-5.9281676367925620 \pm 6.52 \cdot 10^{-14} + \mathrm{i}\left(1.07 \cdot 10^{-13} \pm 2.63 \cdot 10^{-14}\right)\right) \cdot \epsilon^{-2} \\
&+ \left(9.86757086818429 \pm 1.64 \cdot 10^{-12} - \mathrm{i}\left(2.54 \cdot 10^{-11} \pm 9.83 \cdot 10^{-12}\right)\right) \cdot \epsilon^{-1} \\
&- 89.066074732329 \pm 8.25 \cdot 10^{-10} + \mathrm{i}\left(8.10892634289 \pm 2.37 \cdot 10^{-9}\right) \\
&+ \mathcal{O}(\epsilon) \,.
\end{aligned}
$$

High loop integrals: 6L bubble

- geometric decomposition
- `minn=10**7`, `transform='baker'`, polysingular fit
- analytic result Kompaniets, Panzer (2017)

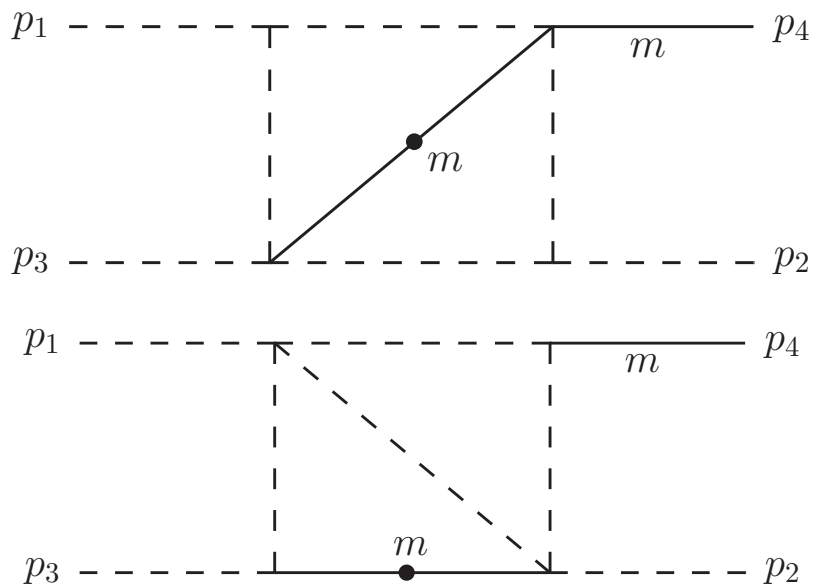


$$B_{6L}^{\text{analyt.}} = \frac{1}{\epsilon^2}\frac{147}{16}\zeta_7 - \frac{1}{\epsilon}\left(\frac{147}{16}\zeta_7 + \frac{27}{2}\zeta_3\zeta_5 + \frac{27}{10}\zeta_{3,5} - \frac{2063}{504000}\pi^8\right) + \mathcal{O}(\epsilon^0)$$
$$= \frac{9.264208985946416}{\epsilon^2} + \frac{91.73175282208716}{\epsilon} + \mathcal{O}(\epsilon^0)\,.$$

$$B_{6L}^{\text{num.}} = +\left(9.2642089624 \pm 1.58 \cdot 10^{-8}\right)\cdot\epsilon^{-2}$$
$$+\left(91.73175426 \pm 2.15 \cdot 10^{-6}\right)\cdot\epsilon^{-1}$$
$$+\left(1118.607204 \pm 1.31 \cdot 10^{-4}\right) + \mathcal{O}(\epsilon)\,.$$

Nbox

- $m_{int} = m_{ext} \rightarrow$ numerically unstable
- Use `split` option to split integration region
- $s = (p_1 + p_2)^2 = -1$, $t = (p_1 + p_3)^2 = -0.8$, $m^2 = 0.1$
- 8 to 11 digits precision

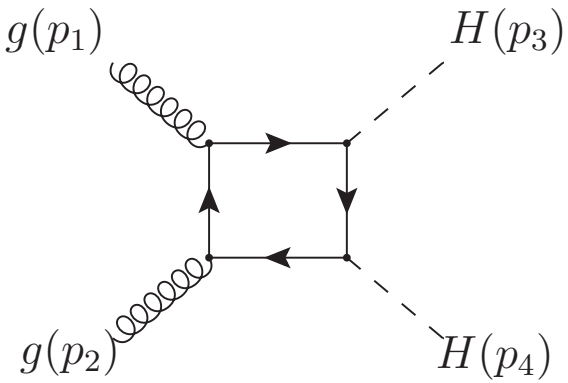


`minn=10**7`, `minn=10**9`, `minn=15173222401`,
`transform='korobov4'`, `transform='korobov6'`, `transform='korobov6'`
polysingular fit for H_a, polysingular fit for H_b, for H_c.

Higgs boson pair production with full top quark mass dependence

$$\sigma^{NLO} = \sigma^{LO} + \sigma^{virt} + \sigma^{real}$$

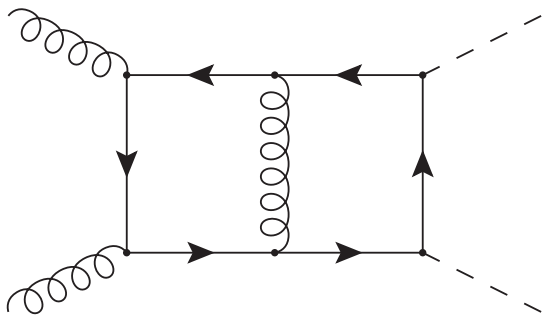
σ^{LO}



analytic result known

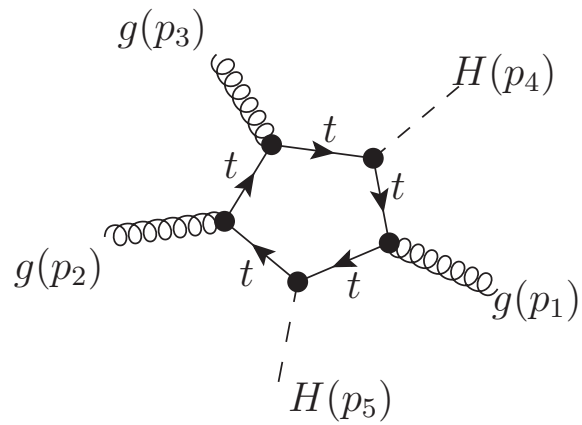
Glover, van der Bij (1988)

σ^{virt}



requires two-loop amplitude

σ^{real}

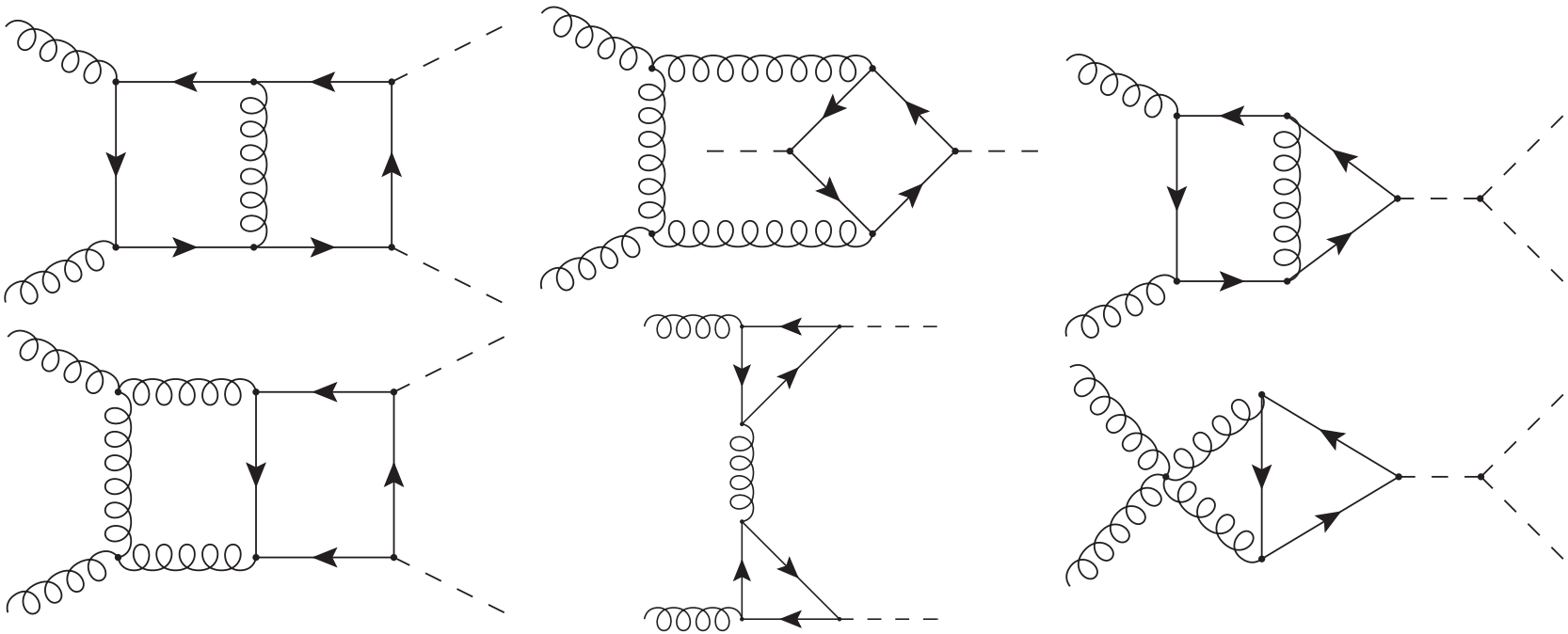


calculated with GoSam-2.0

Dipole subtraction Catani, Seymour (1996) for the cancellation of IR divergences

Gosam: Cullen, Greiner, Heinrich, Luisoni, Mastrolia, Ossola, Reiter, Tramontano (2011), Cullen, van Deurzen, Greiner, Heinrich, Luisoni, Mastrolia, Mirabella, Ossola, Peraro, JS, von Soden-Fraunhofen, Tramontano (2014)

Contributing diagrams



- 2-loop integrals with 4 mass scales $\{\hat{s}, \hat{t}, m_t^2, m_h^2\}$
- Only small subset known analytically:
  - $gg \to h$ Spira et al. (1993); Anastasiou et al. (2006)
  - $h \to Z\gamma$ Gehrmann, Guns, Kara (2015); Bonciani, Del Duca, Frellesvig, Henn, Moriello, Smirnov (2015)
  - Reducible (1-loop)^2 contributions Degrassi, Giardino, Gröber (2016)

Integral reduction

- Integration-by-parts reduction Tkachov (1981), Chetyrkin, Tkachov (1981)
- Choose 5 planar + 3 nonplanar integral families with 9 propagators
- Complete reduction of planar families with Reduze von Manteuffel, Studerus (2012) using numerical values for masses:

$$\{\hat{s}, \hat{t}, m_t^2, m_h^2\} \to \{\hat{s}, \hat{t}, 173^2, 125^2\}$$

- Nonplanar families not fully reduced
- Choose finite integrals where possible von Manteuffel, Panzer, Schabinger (2014)
- Use dimension shift relations Tarasov (1996), Lee (2010)
- Improves stability of numerical integration

Integration

Phase-space

- unweighted events based on LO calculation
- originally computed 917 points, excluded 4 (now 6320)

Amplitude

- Precision for individual sector integrals set dynamically
- Target accuracy F_1 : 3%, F_2 : 5-20%
- GPU time/PS point: 80min - 2d (median 2h)

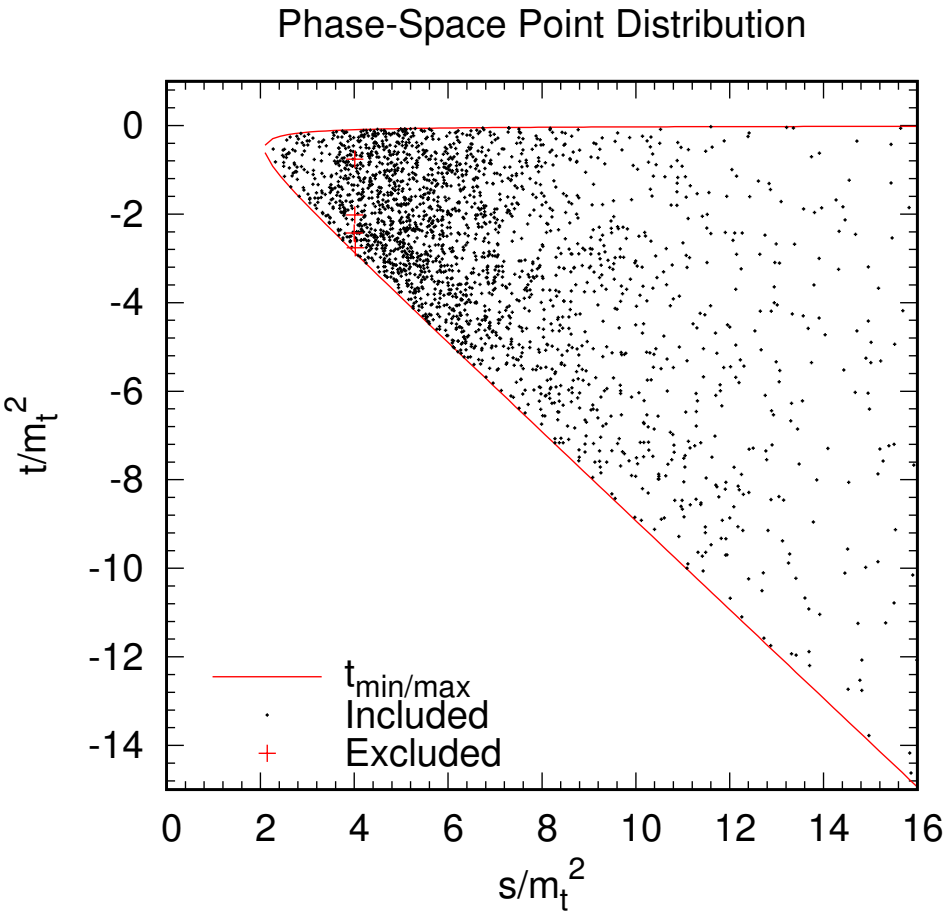


Figure by Stephen Jones

Results - Inclusive cross section

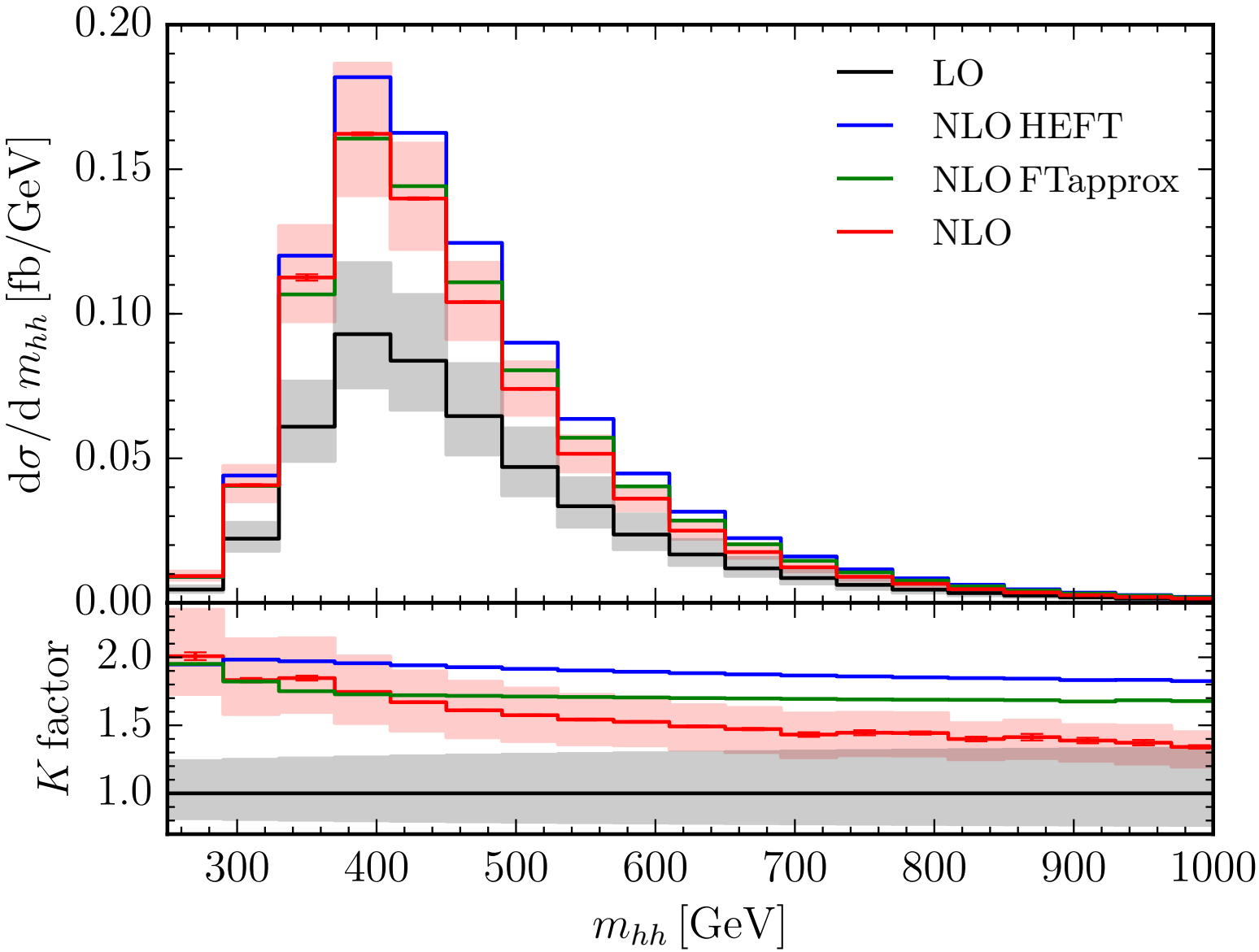
$$\sigma^{NLO}(pp \to hh) = 32.91^{+13.6\%}_{-12.6\%}\,\text{fb} \pm 0.3\%(\text{stat.}) \pm 0.1\%(\text{int.})$$

Borowka, Greiner, Heinrich, Jones, Kerner, JS, Schubert, Zirke (2016), Borowka, Greiner, Heinrich, Jones, Kerner, JS, Zirke (2016)

- LHC@14 TeV
- 7-point scale variation $\mu_{F/R} \in \{\mu_0/2, \mu_0, 2\mu_0\}$ with $\mu_0 = \frac{m_{hh}}{2}$
- PDF4LHC15_nlo_30_pdfas
- $m_h = 125$ GeV, $m_t = 173$ GeV
- agreement with independent result Baglio, Campanario, Glaus, Mühlleitner, Spira, Streicher (2018)

	$\sigma(\sqrt{s} = 14\text{ TeV})$
LO Full	$19.85^{+27.6\%}_{-20.5\%}$ fb
NLO Full	$32.91^{+13.6\%}_{-12.6\%}$ fb
NLO BHEFT	$38.32^{+18.1\%}_{-14.9\%}$ fb
NLO $\text{FT}_{\text{approx}}$	$34.26^{+14.7\%}_{-13.2\%}$ fb

Results - m_{hh}


LO
NLO HEFT
NLO FTapprox
NLO
$\mathrm{d}\sigma/\mathrm{d}\, m_{hh}$ [fb/GeV]
K factor
m_{hh} [GeV]
0.20
0.15
0.10
0.05
0.00
2.0
1.5
1.0
300
400
500
600
700
800
900
1000

Conclusion and Outlook

- Improvements in pySecDec:
  - Quasi Monte Carlo integration
  - GPU support
- NLO Higgs boson pair production with full top quark mass dependence

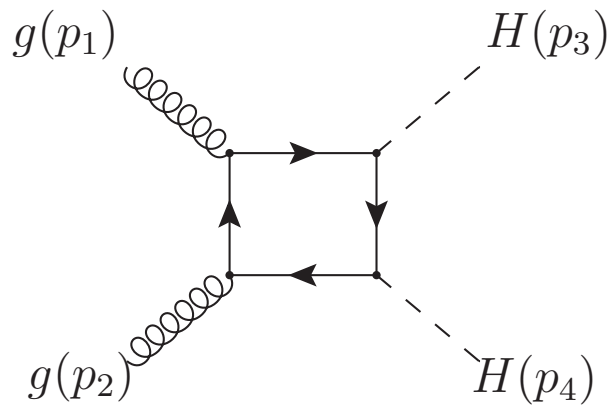
Outlook

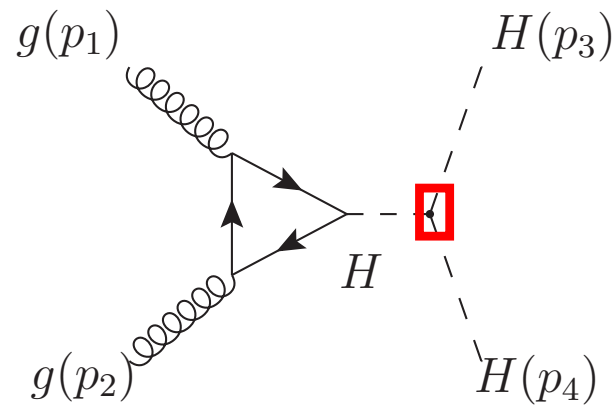
- Apply pySecDec setup to other processes
- Further improvements to pySecDec:
  - Expansion by regions
  - Improvements for integrals with numerators

Backup

NLO Higgs boson pair production in gluon fusion

- (HL-)LHC: Determine Higgs boson properties
- Higgs self-couplings probe Higgs potential and mechanism of EW symmetry breaking





Higgs potential:

$$V(\Phi) = -\mu^2 \Phi^\dagger \Phi + \lambda \left(\Phi^\dagger \Phi\right)^2$$

$$V(h) = \frac{m_h^2}{2} h^2 + \frac{m_h^2}{2v} h^3 + \frac{m_h^2}{8v^2} h^4$$

The process $gg \to hh$

- LO (1-loop) with full top quark mass dependence Glover, van der Bij (1988)
- NLO in $m_t \to \infty$ limit (HEFT) Dawson, Dittmaier, Spira (HPAIR 1998)
  - $+ \frac{1}{m_t}$ expansion Grigo, Hoff, Melnikov, Steinhauser (2013); Grigo, Hoff, Steinhauser (2015)
  - + full m_t dependence in real radiation ($\mathrm{FT}_{\mathrm{approx}}$) Maltoni, Vryonidou, Zaro (2014)
- NNLO in $m_t \to \infty$ limit De Florian, Mazzitelli (2013)
  - + matching coefficients Grigo, Hoff, Melnikov, Steinhauser (2013)
  - $+ \frac{1}{m_t}$ expansion Grigo, Hoff, Steinhauser (2015)
  - + resummation Shao, Li, Li, Wang (2013), de Florian, Mazzitelli (2015)
  - fully differential de Florian, Grazzini, Hanga, Kallweit, Lindert, Maierhöfer, Mazzitelli, Rathlev (2016)
  - real-virtual $\frac{1}{m_t}$ expansion Davies, Herren, Mishima, Steinhauser (2019)
- NLO in high energy limit Davies, Mishima, Steinhauser (2019)
- NLO (2-loop) with full top quark mass dependence Borowka, Greiner, Heinrich, Jones, Kerner, JS, Schubert, Zirke (2016), Borowka, Greiner, Heinrich, Jones, Kerner, JS, Zirke (2016) Baglio, Campanario, Glaus, Mühlleitner, Spira, Streicher (2018)

- Transverse momentum resummation Ferrera, Pires (2016), Threshold resummation de Florian, Mazitelli (2018)
- Parton shower matching Heinrich, Jones, Kerner, Luisoni, Vryonidou (2017) Jones, Kuttimalai (2017)
- Pade approximation Groeber, Maier, Rauh (2017), $p_T^2 + m_h^2$ expansion Bonciani, Degrassi, Giardino, Groeber (2018)
- Combination with NNLO in $m_t \to \infty$ Grazzini, Heinrich, Jones, Kallweit, Kerner, Lindert, Mazzitelli (2018),
- EFT studies Buchalla, Capozi, Celis, Heinrich, Lybocz (2018)
- Self coupling studies with PS Heinrich, Jones, Kerner, Luisoni, Scyboz (2019)
- Quartic Higgs coupling Bizon, Haisch, Rottoli (2018), Borowka, Duhr, Maltoni, Pagani, Shivaji, Zhao (2019)
- Combination with high energy approximation Davies, Heinrich, Jones, Kerner, Mishima, Steinhauser, Wellmann (2019) ($\to$ talk by Stephen Jones)