Computer Algebra Challenges for Precision Calculations

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Anatomy of precision calculations

- Perturbation theory expansion
  - scattering amplitudes for real and virtual corrections
  - subtraction scheme to extract and cancel singular configurations
  - universal anomalous dimensions for resummation
    - DGLAP evolution of parton distributions
    - soft-gluon resummation
    - resummation of large logarithms: p_T, N-jettiness, R, ...

- Require (ideally analytic) computation of loop and phase space integrals

Multi-loop integrals

- Calculation of loop or phase space integrals
  - phase space: cut loop integral
  - expressed in generic loop integrals (here: two-loop)

$$I_{t,r,s}(p_1,\ldots,p_n) = \int \frac{d^d k}{(2\pi)^d} \frac{d^d l}{(2\pi)^d} \frac{1}{D_1^{m_1}\ldots D_t^{m_t}} S_1^{n_1}\ldots S_q^{n_q}$$

- Two challenges
  - algebraic complexity
    - reduce large number of loop integrals to smaller set of master integrals
  - analytic complexity
    - evaluate master integrals (analytically or numerically)

Multi-loop integrals

- Reduction to master integrals: integration-by-part (IBP) equations

$$\int \frac{d^d k}{(2\pi)^d} \frac{d^d l}{(2\pi)^d} \frac{\partial}{\partial a^\mu} \left[b^\mu f(k,l,p_i) \right] = 0 \qquad \text{with } a^\mu = k^\mu, l^\mu; b^\mu = k^\mu, l^\mu, p_i^\mu$$

  - yield large system of linear relations among integrals (up to millions of equations)
- Method of solution
  - closed form
  - iterative with lexicographic ordering (Laporta algorithm: Reduze, FIRE, Kira, LiteRed,...)
- Result
  - generic integrals as linear combinations of a small number of master integrals

Multi-loop integrals

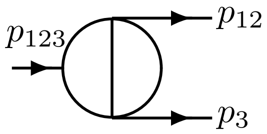
- Evaluation of master integrals
  - integrals are typically IR and/or UV divergent
- Direct numerical evaluation: sector decomposition (T.Binoth, G.Heinrich)
  - Partition of integration space into sectors of non-overlapping singularities
  - Laurent expansion of integrand

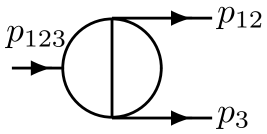
$$(1-z)^{-1-\epsilon} = -\frac{1}{\epsilon}\delta(1-z) + \sum_n \frac{(-\epsilon)^n}{n!}\left(\frac{\ln^n(1-z)}{1-z}\right)_+$$

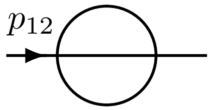
  - Numerical sector integrals: pySecDec, FIESTA
- Direct analytical evaluation: Mellin-Barnes, Feynman parameters
- Indirect analytical evaluation: differential equations

Multi-loop integrals

- Differential equations for master integrals (A.Kotikov; E. Remiddi, TG)
  - differentiate integrand with respect to masses or momenta
  - apply IBP identities

$$s_{123}\frac{\partial}{\partial s_{123}}$$


$$= \frac{d-4}{2}\,\frac{2s_{123}-s_{12}}{s_{123}-s_{12}}$$


$$-\frac{3d-8}{2}\,\frac{1}{s_{123}-s_{12}}$$


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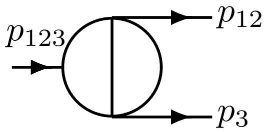
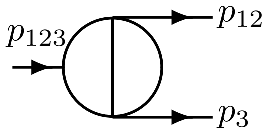
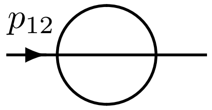
$$s_{12}\frac{\partial}{\partial s_{12}}$$


$$= -\frac{d-4}{2}\,\frac{s_{12}}{s_{123}-s_{12}}$$


$$+\frac{3d-8}{2}\,\frac{1}{s_{123}-s_{12}}$$


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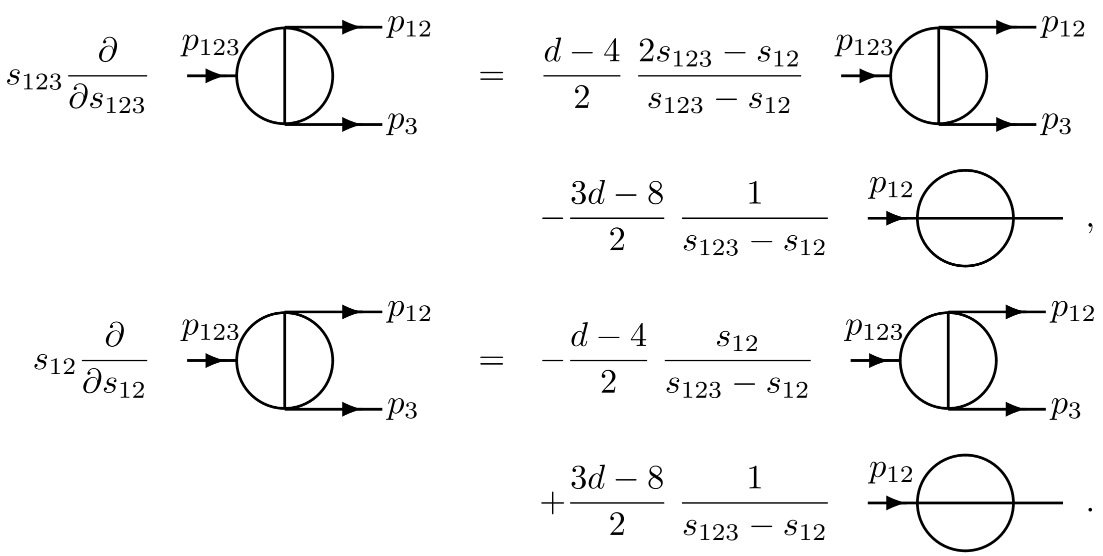
  - integrate differential equations and match boundary conditions

Multi-loop integrals

- Systematic solution of DE
  - d-log form (J. Henn)
  - alphabet of process (letters = denominators)
  - iterated integrals
  - solutions: generalized polylogarithms (GPL)



$$
\mathrm{G}(w_1,\ldots,w_n;z) = \int_0^z \frac{dt}{t-w_1}\mathrm{G}(w_2,\ldots,w_n;t)
$$

- Requires
  - derivation of differential equations: IBPs
  - analytic expression for NxN matrix of differential equations for N masters
  - optimized choice of master integrals: decoupling, diagonalization

Multi-loop integrals in practise

- Main bottleneck: IBP equations

$$I_{t,r,s}(p_1,\ldots,p_n) = \int \frac{d^dk}{(2\pi)^d}\frac{d^dl}{(2\pi)^d}\frac{1}{D_1^{m_1}\ldots D_t^{m_t}} S_1^{n_1}\ldots S_q^{n_q}$$

  - t: number of different propagators
  - r: mass dimension of denominator (r ≥ t)
  - s: mass dimension of numerator
- Examples at current frontier: $10^{6..7}$ integrals to $10^{2..3}$ master integrals
  - three-loop 2 → 2 amplitudes: 4 ≤ t ≤ 10, t ≤ r ≤ 10, s ≤ 6
  - four-loop OME for splitting functions: 5 ≤ t ≤ 15, t ≤ r ≤ 15, s ≤ 6
  - differential equations for master integrals: same (t,r), typically s ≤ 2
- Combinatorial explosion of IBP system size

Multi-loop integrals in practise

- Classical approach to IBP solutions: Laporta algorithm
  - IBP codes (Reduze, FIRE, Kira, LiteRed,...) use MPI for parallelization
  - run typically on multi-core machines with ~TB of RAM
  - distribute subsystems on different threads
  - limitations: memory usage per thread, interconnection of subsystems

- Algebraic complexity
  - critically depends on number of scales (space-time dimension *d*, masses, invariants)
  - large-scale algebraic simplifications at intermediate stages or as final step (polynomial arithmetic, using external tools: Fermat, Ginac, Symbolica)
  - size of results (reduction tables, after simplification): can be TBs, insertion time-consuming

Multi-loop integrals in practise

- Improvement to IBP reduction: syzygy equations (J.Gluza, D.Kosower, K.Larsen)
  - taming combinatorial growth: select IBP seed equations to always have r = t
  - must derive syzygy equations for each integral topology: poor automation
- Finite field methods (A. von Manteuffel, R.Schabinger; T. Peraro)
  - solve IBP system for multiple integer values of *d*, masses and invariants (or subset)
  - perform integer arithmetic modulo some large number
  - full workflow can be done on finite field
  - reconstruct all rational coefficients in solution (FiniteFlow, Kira, FinRed)
- Challenges with finite field methods
  - point of reconstruction: IBP tables, integral coefficients, GPL coefficients
  - number of evaluations required for reconstruction and validation
  - inversion of rational matrices as task: could profit from novel computer architectures

Multi-loop integrals in practise

- Limitation of algebraic approaches: number of mass scales (internal masses)
  - Complexity of IBPs and DEs (size of alphabet ~ number of possible kinematical cuts)
  - IBP reduction often not feasible, neither for amplitude nor for differential equation
- Numerical approach to IBP
  - IBP reduction and derivation of DE for each set of fixed numerical masses and kinematics
  - repeated for each phase space point (timing)
  - for symbolic *d*, truncated to finite terms in $\varepsilon = (4-d)/2$
  - integer arithmetic
- Numerical approach to high-precision solutions to DE
  - solution by asymptotic series: DiffExp, SeaSyde
    (M.Hidding; T.Armadillo, R. Bonciani, S. Devoto, N. Rana, A. Vicini)
  - differential equations in complex mass parameter (Feynman $+i\delta$): AMFlow (X. Lui, Y.Q. Ma)

Summary

Main bottleneck in calculation of loop amplitudes: solution of IBPs

- express loop amplitudes as linear combination of master integrals
- prerequisite for computation of master integrals from differential equations
- Task: solve large systems of linear equations with rational coefficients

Approaches

- symbolic solution: Laporta algorithm (+ syzygy) (+ finite field reconstruction)
- numerical solution: IBP and DE solution for each phase space point

Computing challenges

- problem size often memory and storage limited
- hardware solutions for large linear systems
- parallelization at different stages