Numerical multi-loop integration on heterogeneous many-core processors

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Outline

1. Loop integral
2. Multivariate integration/Lattice rules
   - Lattice rules
   - Periodizing transformations
3. Loop diagrams
4. Architecture
   - GPU
   - Suiren2/PEZY-SC2
5. Results
   - GPU results
   - PEZY results
6. Conclusions

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Higher order corrections are required for accurate theoretical predictions of the cross-section for particle interactions. Loop diagrams are taken into account, leading to the evaluation of loop integrals — for which analytic integration is not generally possible.

The goal is to perform accurate loop integral computations; and to develop computer programs which evaluate multi-loop Feynman integrals numerically/directly.

Previously in [7, 10, 6], we reported precise numerical results for 2-, 3- and 4-loop Feynman integrals using adaptive multi-dimensional integration and linear extrapolation. In [4, 5] we handle 2- and 3-loop integrals with (transformed) lattice rules on GPUs.

Here we use composite lattice rules (with transformation) for 3- and 4-loop integrals, and parallel execution on systems with GPU or PEZY accelerators.
Loop integral - Representation

$L$-loop integral with $N$ internal lines

$$
\mathcal{F} = \frac{\Gamma \left( N - \frac{\nu L}{2} \right)}{(4\pi)^{\nu L/2}} (-1)^N \int_0^1 \prod_{r=1}^N dx_r \delta(1 - \sum x_r) \frac{C^{N-\nu(L+1)/2}}{(D - i\varrho C)^{N-\nu L/2}}
$$

$C$ and $D$ are polynomials determined by the topology of the corresponding diagram and physical parameters; $\nu$ is the space-time dimension (i.e., $= 4$ unless used for regularization); $\varrho = 0$ unless $D$ vanishes in the domain.
Figure: [MC-QMC] (left) 300 random points; (right) 300 points of 2-dimensional lattice constructed with generator vector $z = (1, 129)$ [1]

Monte Carlo (MC): $I = \int_{C_d} f(x) \, dx \approx Qf = \frac{1}{n} \sum_{j=0}^{n-1} f(x_j)$

where $x_j$ are uniform random, and the error $|Qf - I| \sim O(1/\sqrt{n})$ as $n \to \infty$

Quasi-Monte Carlo (QMC), equidistributed rules, e.g., (good) lattice rules [3, 20]: the points $x_j$ are generated on a (good) lattice in the half-open cube $U_d = [0, 1)^d$; with favorable convergence properties (compared to MC), particularly for smooth, 1-periodic
Extension of 1D rectangle rule: \( Rf = \frac{1}{n} \sum_{j=0}^{n-1} f\left(\frac{j}{n}\right) \)

Rank-1 lattice rule: \( Q(z, n)f = \frac{1}{n} \sum_{j=0}^{n-1} f\left(\{\frac{j}{n}z\}\right) \)

where \( z \) is an integer generator vector with components \( z \in \mathbb{Z}_n = \{1 \leq z < n, \gcd(z, n) = 1\} \);

\( \{x\} \) denotes the vector in \( \mathcal{U}_d \) obtained by taking the fractional part of each component of \( x \);

classically \( n \) is prime (i.e., \( \mathbb{Z}_n = \{1, 2, \ldots, n-1\} \))
(has been relaxed, cf. [12, 14])
Sample generators

100M, 7D: (1, 41883906, 22682973, 44229424, 29466837, 15518263, 42112409),
100M, 10D: (1, 41883906, 22682973, 44229424, 29466837, 8176047, 49462874, 1162485, 46871525, 36107330),
200M, 7D: (1, 76384079, 93229505, 12830863, 56635299, 54395013, 90891159),
400M, 7D: (1, 155987582, 55105452, 187223455, 109010593, 87245157, 73239020),
400M, 8D: (1, 155987582, 55105452, 187223455, 109010593, 87245157, 122592441, 131361432)

(100M denotes 100,000,007; 200M denotes 200000033; 400M denotes 400,000,009)

Note that projections of higher-dimensional generators can be used in lower dimensions.

We pre-compute the generators \((z_1, \ldots, z_d)\) using the component by component (CBC) algorithm by Nuyens and Cools [13, 14]. The CBC algorithm runs in \(O(d n \log(n))\) time and \(O(n)\) space.
An embedded sequence is given in [20]; with \( m \) copies in \( r \) coordinate directions:

\[
Q_r f = \frac{1}{m^n} \sum_{k_r=0}^{m-1} \cdots \sum_{k_1=0}^{m-1} \sum_{j=0}^{n-1} f \left( \{ \frac{j}{n} \mathbf{z} + \frac{1}{n} (k_1, \ldots, k_r, 0, \ldots, 0) \} \right)
\]

for \( 0 \leq r \leq d \), \( n \) and \( m \) relatively prime, and \( \mathbf{z} \) is a generator vector.

The points of \( Q_{r+1} \) include the points of \( Q_r \) for \( 0 \leq r < d \).

\( Q_r \) has \( m^r n \) points and is of rank \( r \) for \( 1 \leq r \leq d \); \( Q_0 \) is of rank 1.

\( Q_d \) is the \( m^d \)-copy rule.

An error estimate is calculated for \( Q_d \).
Figure: [2D rule $Q_0$] with 11 points, $\mathbf{z} = (1, 4)$
Figure: [2D rule $Q_1$] corresponding to $Q_0$, $\mathbf{z} = (1, 4)$

$Q_1$ includes the points of $Q_0$. 
Figure: [2D rule $Q_2$] corresponding to $Q_0$, $z = (1, 4)$

$Q_2$ includes the points of $Q_0$ and $Q_1$ (embedded sequence), and is the "2$^2$-copy" of $Q_0$. 
Periodizing transformations

The lattice rule is applied after a periodizing transformation of the integrand. We have used transformations (tanh [17], $\sin^m$ [18, 19] that also smoothen singular behavior at the boundaries of the integration domain [4, 5].

Sidi $\sin^m$ transformations for an integral $\mathcal{I}f = \int_0^1 f(x) \, dx$:

$$x = \Psi_m(t) = \frac{\theta_m(t)}{\theta_m(1)}, \quad m = 1, 2, \ldots$$

with $\theta_m(t) = \int_0^t \sin^m(\pi u) \, du$.

$$\Psi_2(t) = t - \sin(2\pi t)/(2\pi), \quad \Psi'_2(t) = 2 \sin^2(\pi t)$$

$$\Psi_4(t) = t + (-8 \sin(2\pi t) + \sin(4\pi t))/(12\pi), \quad \Psi'_4(t) = \frac{8}{3} \sin^4(\pi t)$$

$$\Psi_6(t) = t - (45 \sin(2\pi t) - 9 \sin(4\pi t) + \sin(6\pi t))/(60\pi), \quad \Psi'_6(t) = \frac{16}{5} \sin^6(\pi t)$$
Figure: $\Psi_4$ transformation of $1/\sqrt{x_1 x_2 (1 - x_1)(1 - x_2)}$ over unit square: (a) without; (b) with transformation [4]
Sample 3-loop self-energy diagrams

Figure: [3ls] Sample 3-loop self-energy diagrams, cf. Laporta [11] (Diag. \((r, t, u, v)\) with masses), Baikov and Chetyrkin [2] (Diag. \((L_2, N_0, L_0)\) massless): (a) Diagram \((r/N_2)\) \(N = 7\); (b) Diagram \((t/N_0)\) \(N = 8\); (c) Diagram \((u)\) \(N = 8\); (d) Diagram \((v/L_0)\) \(N = 8\)
Sample 4-loop self-energy diagrams

(a) \hspace{1cm} (b)

**Figure:** [4ls] 4-loop self-energy diagrams with massless internal lines, cf., Baikov and Chetyrkin [2]: (a) Diagram $M44$, $N = 9$; (b) Diagram $M45$, $N = 9$
**GPU: Kepler 20m**  
From DeviceQuery program (NVIDIA), run on a node of thor.cs.wmich.edu:

| Specification                      | Details                        |
|-----------------------------------|--------------------------------|
| CUDA Capability Major/Minor       | 3.5                            |
| Total amount of global memory     | 4800 MBytes (5032706048 bytes) |
| (13) Multiprocessors x (192) CUDA| 2496 CUDA Cores                |
| Cores/MP                          | 706 MHz (0.71 GHz)             |
| GPU Clock rate                    | 2600 Mhz                       |
| Memory Clock rate                 | 320-bit                        |
| Memory Bus Width                  | 1310720 bytes                  |
| L2 Cache Size                     | 65536 bytes                    |
| Total amount of constant memory   | 49152 bytes                    |
| Total amount of shared memory per | 5536                            |
| block                             |                                |
| Total number of registers available per block | 32 |
| Warp size                         | 2048                            |
| Maximum number of threads per multiprocessor | 1024 |
| Integrated GPU sharing Host Memory | No                               |
| Support host page-locked memory mapping | Yes                             |
| Device has ECC support            | Enable                          |
| Device supports Unified Addressing (UVA) | Yes                             |
Suiren2 (ZettaScaler 2.2)

**Figure:** Suiren2 at KEK, liquid immersion cooling, many-core supercomputer
Suiren2 (ZettaScaler 2.2)

From top500.org:
Suiren2 - ZettaScaler-2.2, Xeon D-1571 16C 1.3GHz, Infiniband EDR

- Site: High Energy Accelerator Research Organization /KEK
- System URL: http://www.exascaler.co.jp/
- Manufacturer: PEZY Computing / Exascaler Inc.
- Cores: 762,624
- Memory: 26,112 GB
- Processor: Xeon D-1571 16C 1.3GHz
- Interconnect: Infiniband EDR
- Linpack Performance: Rmax: 797.994 TFlop/s; Nmax: 1,238,016
- Theoretical Peak: Rpeak: 1,082.57 TFlop/s
- Power Consumption: Power: 47.40 kW (Submitted)

Configuration at KEK:
- 6 tanks
- 2 bricks (high density server boards) per tank
- total bricks is $6 \times 2 = 12$
- 4 nodes per brick, 8 PEZY-SC2 boards per node
- total $8 \times 4 = 32$ PEZY-SC2 accelerator boards per brick
- total number of nodes: $4 \times 12 = 48$
- total number of PEZY-SC2 boards: $48 \times 8 = 384$
Suiren2 (ZettaScaler 2.2)

**Figure:** Suiren2 node configuration
MIMD manycore PEZY-SC2 processor [21]

Some specifications:

- **Frequency**: 1GHz
- **Cache Memory (Chip Total)**: L1: 4MB(D), 8MB(I), L2: 8MB(D), 4MB(I) LLC: 40MB
- **Local Memory**: Total 40MB (20KB/PE)
- **PE**: 2,048 (1986) core 2 issue/cycle
- **8 way time-sliced fine-grain multi-threading**: (Total: 16,384 threads)
- **Peak Performance**: 8.2TFLOPS(SP), 4.1TFLOPS(DP), 16.4TFLOPS(HP)
- **Power**: 180W (Peak Estimated)
Programming model [21]

- PZCL environment: program consists of a CPU (host) program in C++ and kernel in OpenCL
- CPU code: sets up kernel code and buffers, initializes buffers allocated in PEZY-SC2, and invokes kernel code on PEZY-SC2 as multiple threads
- threads can run independently on MIMD PEZY-SC2 processor
- program can be generated by Goose compiler [8, 9]
- Goose uses compiler directives (pragmas) similar to OpenMP [16] and OpenACC [15]
### (Simple) LR integration for 3-loop massive self-energy diagrams on GPU

| Diagram   | $N$ | # Points $n$ | Result       | Error      | Time [s] |
|-----------|-----|--------------|--------------|------------|----------|
| Fig [3ls] (r) | 7   | 200M         | 1.34139904258 | 1.99 e-07 | 0.616    |
|           |     | 350M         | 1.34139953791 | 2.96 e-07 | 1.080    |
|           |     | Exact:       | 1.34139924145 |           |          |
| Fig [3ls] (t) | 8   | 200M         | 0.27960944661 | 5.23 e-07 | 0.749    |
|           |     | 350M         | 0.27960937820 | 4.55 e-07 | 1.314    |
|           |     | Exact:       | 0.27960892328 |           |          |
| Fig [3ls] (u) | 8   | 200M         | 0.18262710188 | 1.36 e-07 | 0.752    |
|           |     | 350M         | 0.18262769916 | 4.62 e-07 | 1.317    |
|           |     | Exact:       | 0.18262723754 |           |          |
| Fig [3ls] (v) | 8   | 200M         | 0.14801298928 | 3.15 e-07 | 0.740    |
|           |     | 350M         | 0.14801307409 | 2.30 e-07 | 1.299    |
|           |     | Exact:       | 0.14801330396 |           |          |

**Table:** (Simple) LR integration for 3-loop massive self-energy diagrams on GPU [4, 5]
(\(m = 1, 2\)) LR results for 3-loop massive self-energy diagrams on GPU

| DIAGRAM      | N | # PTS | \(m\) | RESULT                  | ABS. ERR. | TIME [s] |
|--------------|---|-------|-------|-------------------------|-----------|----------|
| Fig [3ls] (t) | 8 | 400M  | 1     | 0.2796089827126         | 5.94 e-08 | 0.999    |
|              |   |       | 2     | 0.2796089232826         | 2.52 e-14 | 127.8    |
| \(5^{13} (7D)\) | 1 |       |       | 0.2796089226167         | 6.66 e-10 | 3.047    |
|              |   |       | 2     | 0.2796089232824         | 1.63 e-13 | 390.1    |
| Exact:       |   |       |       | 0.2796089232826         |           |          |
| Fig [3ls] (u) | 8 | 400M  | 1     | 0.1826272683315         | 3.08 e-08 | 1.001    |
|              |   |       | 2     | 0.1826272375394         | 2.18 e-13 | 128.1    |
| \(5^{13} (7D)\) | 1 |       |       | 0.1826272372834         | 2.56 e-10 | 3.054    |
|              |   |       | 2     | 0.1826272375391         | 1.46 e-13 | 391.0    |
| Exact:       |   |       |       | 0.1826272375392         |           |          |
| Fig [3ls] (v) | 8 | 400M  | 1     | 0.1480133458323         | 4.19 e-08 | 1.558    |
|              |   |       | 2     | 0.1480133039588         | 2.37 e-13 | 199.4    |
| \(5^{13} (7D)\) | 1 |       |       | 0.1480133033037         | 6.55 e-10 | 4.752    |
|              |   |       | 2     | 0.1480133039581         | 3.46 e-13 | 608.1    |
| \((15 \rightarrow 7D)\) | 1 |       |       | 0.1480133034035         | 5.55 e-10 | 4.751    |
|              |   |       | 2     | 0.1480133039583         | 8.97 e-14 | 608.6    |
| Exact:       |   |       |       | 0.1480133039584         |           |          |

**Table:** \((m = 1, 2)\) LR results for 3-loop massive self-energy diagrams on GPU
(m = 1, 2) LR results for 4-loop massless self-energy diagrams on GPU

| Diagram          | N  | # Pts | m   | Result  | Abs. Err. | Rel. Err. | Time [s] |
|------------------|----|-------|-----|---------|-----------|-----------|----------|
| Fig [4ls] (M44)  | 9  | 100M  | 1   | 55.657754 | 7.25 e-02 | 1.30 e-03 | 0.430    |
|                  |    |       | 2   | 55.586092 | 8.38 e-04 | 1.51 e-05 | 113.4    |
|                  |    | 400M  | 1   | 55.600351 | 1.51 e-02 | 2.72 e-03 | 1.770    |
|                  |    |       | 2   | 55.585416 | 1.62 e-04 | 2.91 e-06 | 452.9    |
|      5^{13} (15 → 8D) | 1 |      |     | 55.577700 | 7.55 e-03 | 1.36 e-04 | 5.400    |
|                  |    |       | 2   | 55.585135 | 1.19 e-04 | 2.14 e-06 | 1382     |
| Exact:           |    |       |     | 55.585254 |           |           |          |
| Fig [4ls] (M45)  | 9  | 100M  | 1   | 52.058688 | 4.08 e-02 | 7.85 e-04 | 0.450    |
|                  |    |       | 2   | 52.018436 | 5.67 e-04 | 1.09 e-05 | 114.9    |
|                  |    | 400M  | 1   | 52.014437 | 1.43 e-03 | 6.96 e-05 | 1.794    |
|                  |    |       | 2   | 52.017790 | 7.92 e-05 | 1.52 e-06 | 459.4    |
|      5^{13} (15 → 8D) | 1 |      |     | 52.012072 | 5.80 e-03 | 1.11 e-04 | 5.474    |
|                  |    |       | 2   | 52.017807 | 6.17 e-05 | 1.19 e-06 | 1402     |
| Exact:           |    |       |     | 52.017869 |           |           |          |

Table: (m = 1, 2) LR results for 4-loop massless self-energy diagrams on GPU
\( (m = 2) \) 400M pts. LR results for 3-loop massive self-energy diagram \((u)\) on Suiren2

| DIAGRAM | \( N \) | \#PTS. \( n \) | TIMES [s] ON Suiren2, nXTY: X NODES, Y TASKS |
|---------|-------|-------------|---------------------------------------------|
|         |       |             | 1 node | 2 nodes | 4 nodes | 8 nodes |
| Fig [3ls] \((u)\) | 8 | 400M | n1t1: 140.8 | n2t1: 73.73 |
|         |     |         | n1t2: 71.55 | n2t2: 37.04 |
|         |     |         | n1t4: 36.71 | n2t4: 18.97 |
|         |     |         | n1t8: 19.21 | n2t8: 10.01 |

**Table:** \( (m = 2) \) 400M results for 3-loop massive self-energy diagram \((u)\) on Suiren2; Abs. err. = 4.28e-11; Loop blocks of size 128 \( \times \) 32; Compare to GPU: 128.1 s
\((m = 2) \ 5^{13}\) pts. LR results for 3-loop massive self-energy diagram \((u)\) on Suiren2

| DIAGRAM | N | #PTS. | TIMES [s] on SUIREN2, nXtY: X NODES, Y TASKS |
|---------|---|-------|---------------------------------------------|
| Fig [3ls] \((u)\) | 8 | \(5^{13}\) | n1t1: 433.4, n1t2: 219.8, n1t4: 112.0, n1t8: 57.73 |
|          |   |       | n2t1: 218.4, n2t2: 110.3, n2t4: 56.72, n2t8: 30.14 |
|          |   |       | n4t1: 112.1, n4t2: 56.66, n4t4: 29.74, n4t8: 16.74 |
|          |   |       | n8t1: 56.33, n8t2: 29.05, n8t4: 15.90, n8t8: 9.899 |

**Table:** \((m = 2) \ 5^{13}\) pts. \((7D)\) results for 3-loop massive self-energy diagram \((u)\) on Suiren2; Abs. err. = 4.24e-11; Loop blocks of size 128 \(*\ 32\); **Compare to GPU: 391.0 s**
(m = 2) 400M pts. LR results for 3-loop massless self-energy diagram L0 on Suiren2

| Diagram | N | #Pts. n | TIMES [s] on SUIREN2, nXtY: X nodes, Y tasks |
|---------|---|---------|---------------------------------------------|
| Fig [3ls] (t) | 8 | 400M | n1t1: 143.0 | n1t2: 71.53 | n1t4: 36.66 | n1t8: 19.01 |
|          |   |        | n2t1: 71.52 | n2t2: 36.61 | n2t4: 18.92 | n2t8: 10.09 |
|          |   |        | n4t1: 36.58 | n4t2: 18.87 | n4t4: 9.860 | n4t8: 5.674 |
|          |   |        | n8t1: 18.72 | n8t2: 9.846 | n8t4: 5.456 | n8t8: 3.471 |

**Table:** (m = 2) 400M results for 3-loop massless self-energy diagram L0 on Suiren2; Abs. err. = 8.98e-07, Rel. err. = 4.33e-08; Loop blocks of size 128 * 32; **Compare to GPU: 128.0 s**
(m = 2) $5^{13}$ pts. LR results for 3-loop massless self-energy diagram $L_0$ on Suiren2

| DIAGRAM     | $N$ | #Pts. $n$ | TIMES [s] on SUIREN2, nXtY: X NODES, Y TASKS |
|-------------|-----|-----------|-------------------------------------------|
| Fig [3ls] (t) | 8  | $5^{13}$  | n1t1: 432.7                                |
|             |    |           | n1t2: 217.8                                |
|             |    |           | n1t4: 111.7                                |
|             |    |           | n1t8: 58.33                                |
|             |    |           | n2t1: 217.7                                |
|             |    |           | n2t2: 111.4                                |
|             |    |           | n2t4: 57.58                                |
|             |    |           | n2t8: 30.68                                |
|             |    |           | n4t1: 112.0                                |
|             |    |           | n4t2: 56.58                                |
|             |    |           | n4t4: 29.70                                |
|             |    |           | n4t8: 16.70                                |
|             |    |           | n8t1: 56.23                                |
|             |    |           | n8t2: 29.01                                |
|             |    |           | n8t4: 15.91                                |
|             |    |           | n8t8: 9.857                                |

**Table:** (m = 2) $5^{13}$ pts. (7D) results for 3-loop massless self-energy diagram $L_0$ on Suiren2; Abs. err. = 1.71e-07, Rel. err. = 8.22e-09; Loop blocks of size 128 * 32; Compare to GPU: 390.6 s
$(m = 2)$ LR results for 4-loop massless self-energy diagram $M44$ on Suiren2

| Diagram       | $N$ | #Pts. $n$ | TIMES [s] on SUIREN2, nXtY: X NODES, Y TASKS |
|---------------|-----|-----------|---------------------------------------------|
|               |     |           | 1 node                                      |
|               |     |           | 2 nodes                                     |
|               |     |           | 4 nodes                                     |
|               |     |           | 8 nodes                                     |
| Fig [4ls] M45 | 9   | 400M      | n1t1: 332.5                                 |
|               |     |           | n1t8: 43.32                                 |
|               |     |           | n2t8: 22.36                                 |
|               |     |           | n4t8: 11.90                                 |
|               |     |           | n8t8: 6.711                                 |
| Fig [4ls] M45 | 9   | $5^{13}$  | n2t8: 68.58                                 |
|               |     |           | n4t8: 35.82                                 |
|               |     |           | n8t8: 19.49                                 |

**Table:** $(m = 2)$ results for 4-loop massless self-energy diagram $M45$ on Suiren2; Loop blocks of size $128 \times 32$; 400M pts.: Abs. err. = 2.57e-05, Rel. err. = 4.94e-07, Compare to 400M pts. GPU time: 459.5 s; $5^{13}$ pts.: Abs. err. = 1.02e-06, Rel. err. = 1.95e-08, Compare to $5^{13}$ pts. GPU time: 1402 s
A parallel composite/embedded lattice rule method is presented for the calculation of Feynman loop integrals, using a periodizing transformation that deals with singularities at the boundaries of the integration domain.

The algorithm is implemented in CUDA C (for GPU accelerator) and in C++ with Goose (for PEZY Exascaler accelerator).

Test results are given for classes of 3- and 4-loop self-energy loop diagrams, with or without masses, and using simple \((m = 1)\) and composite \((m = 2)\) lattice rules.

The accuracy improves considerably from \((m = 1)\) to \((m = 2)\) and supersedes that of adaptive parallel integration with the ParInt package for these problems.

The execution times are decreased considerably on the Exascaler system, using multiple PEZY accelerators per node and multiple nodes. The programs incorporate Goose and MPI, and run unchanged on different configurations.
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