Comparison of methods for the calculation of the real dilogarithm regarding instruction-level parallelism

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Abstract

We compare different methods for the computation of the real dilogarithm regarding their ability for using instruction-level parallelism when executed on appropriate CPUs. As a result we present an instruction-level-aware method and compare it to existing implementations.

1 Introduction

The dilogarithm [1] is a special function, which appears in many physics applications, for example in the calculation of quantum corrections in quantum field theory. The investigation of new models beyond the Standard Model of particle physics with large parameter spaces require the numerical evaluation of the dilogarithm (and other functions) billions of times. Such investigations thus require a fast evaluation of the dilogarithm. In the past many time-efficient algorithms have been developed (see e.g. [2–5]) and many are implemented, for example, in general-purpose physics and mathematics program libraries [6–8].

Many of the publicly available implementations, e.g. [6, 7], use formulations for the approximation of the dilogarithm with a strictly sequential execution of floating-point operations. Here the development of modern CPUs with support for instruction-level parallelism (ILP) opens the opportunity for a further reduction of the run-time of the calculation of the dilogarithm. To make use of ILP, the algorithm to calculate the dilogarithm must be formulated appropriately in order to allow for the simultaneous execution of multiple floating-point operations. In this paper a method for the calculation of the real dilogarithm \( \text{Li}_2 \) is presented, which makes use of ILP, resulting in a reduced run-time compared to many algorithms presented so far, when executed on appropriate CPUs.

This paper is organized as follows: In Section 2 different implementation strategies are discussed using a toy example function. In Section 3 an ILP-aware method for the numerical calculation of the dilogarithm is presented. A C implementation of this method can be found in the appendix and in the arXiv submission of this paper.

2 Implementation strategies

As a toy example we consider the real function \( \ln(1+x) \) for \( x > -1 \), which has the Taylor expansion

\[
\ln(1 + x) \approx x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \frac{x^5}{5} - \frac{x^6}{6} + \frac{x^7}{7} \tag{1}
\]

around \( x = 0 \) for \( x \in (-1, 1) \). In Eq. (1) terms of \( O(x^8) \) and beyond have been omitted for brevity. In the following we will briefly show various possible implementations of this function and discuss their performance implications. For brevity we will restrict ourselves to \( x \in (-1, 1) \). In C the function in Eq. (1) could be implemented very naively as follows:

```c
double log1p_naive(double x) {
    return x - 1./2.*x*x + 1./3.*x*x*x
        - 1./4.*x*x*x*x + 1./5.*x*x*x*x*x
        - 1./6.*x*x*x*x*x*x + 1./7.*x*x*x*x*x*x*x*x;
}
```

This naive implementation requires 27 floating-point multiplications and 6 floating-point additions. Although all summands in this implementation can in principle be calculated in parallel, the cost of the many (redundant) floating-point multiplications is usually so high that this formulation is in total very time-inefficient.
As is well known, the performance of this naive implementation can be improved by applying Horner’s scheme [9], which reduces the number of expensive floating-point multiplications to 7 and requires 6 additions:

\[ \ln(1 + x) \approx x \left\{ 1 + x \left[ 1 + x \left( \frac{1}{3} + x \left( -\frac{1}{4} \right) \right) \right] \right\}. \quad (2) \]

A C implementation using Horner’s scheme could read:

```c
double log1p_horner(double x) {
    return x * (1 + x * (-1. / 2 + x * (1. / 3)
        + x * (-1. / 4 + x * (1. / 5)
        + x * (-1. / 6 + 1. / 7 * x))));
}
```

Note that the formulation using Horner’s scheme requires the evaluation of the floating-point operations in strictly sequential order. However, the significant reduction of the number of floating-point multiplications, compared to the naive implementation from above, usually results in a shorter run-time.

There are several different possibilities to reduce the run-time of Horner’s method by rewriting the series expansion of \( \ln(1 + x) \) such that more terms can be calculated in parallel, while the number of floating-point operations is still kept small. One possibility is to split the r.h.s. of Eq. (2) into two distinct sums, one containing the even powers and the other containing the odd powers of \( x \),

\[
\ln(1 + x) \approx x \left\{ 1 + y \left[ \frac{1}{3} + y \left( \frac{1}{5} + \frac{y}{7} \right) \right] \right\} 
- y \left[ \frac{1}{2} + y \left( \frac{1}{4} + \frac{y}{6} \right) \right], \quad (3)
\]

where \( y = x^2 \). This formulation requires 8 floating-point multiplications and 6 additions, i.e. one more multiplication than Horner’s scheme. However, in Eq. (3) both sums can be calculated in parallel, leading to a potential speed-up if the cost of the additional multiplication is smaller than the gain by the parallel execution. A C implementation could read:

```c
double log1p_split(double x) {
    const double y = x * x;
    return x * (1 + y * ((1. / 3 + y * (1. / 5 + 1. / 7 * y)) - y * (1. / 2 + y * (1. / 4 + 1. / 6 * y))));
}
```

Another possibility is to rewrite the r.h.s. of Eq. (1) using Estrin’s scheme [10],

\[
\ln(1 + x) \approx x + y \left( \frac{x}{3} - \frac{1}{2} \right) 
+ z \left[ \frac{x}{5} - \frac{1}{4} + y \left( \frac{x}{7} - \frac{1}{6} \right) \right], \quad (4)
\]

where \( y = x^2 \) and \( z = y^2 \). This form also requires 8 floating-point multiplications and 6 additions, as in Eq. (3). However, in Estrin’s form more terms can be executed in parallel, leading to a potential further speed-up. A C implementation using Estrin’s scheme could read:

```c
double log1p_estrin(double x) {
    const double y = x * x;
    const double z = y * y;
    return x + y * ((1. / 3 * x - 1. / 2) + z * (1. / 5 * x - 1. / 4 + y * (-1. / 6 + 1. / 7 * x)));
}
```

Another option to exploit ILP is to use a rational function approximation, such as a Padé approximant [11], where the numerator and the denominator can be calculated in parallel. A Padé approximant of \( \ln(1 + x) \) at the same order as Eq. (1) can be written as

\[
\ln(1 + x) \approx x + \frac{1 + 51064 \cdot 40143 \cdot x + 44320 \cdot 40143 \cdot x^2 + 320 \cdot 40143 \cdot x^3}{1 + 23712 / 13381 \cdot x + 12320 / 40143 \cdot x^2 + 40143 / 40143 \cdot x^3}, \quad (5)
\]

\[
= x + \frac{1 + 51064 \cdot 40143 \cdot x + 44320 \cdot 40143 \cdot x^2 + 320 \cdot 40143 \cdot x^3}{1 + 23712 / 13381 \cdot x + 12320 / 40143 \cdot x^2 + 40143 / 40143 \cdot x^3}, \quad (6)
\]

where \( y = x^2 \). In Eq. (6) the numerator and the denominator have been re-written using Estrin’s scheme to reduce the number of floating-point multiplications compared to Eq. (5), while still allowing for some degree of ILP at the same time. A C implementation of Eq. (6) could read:

```c
double log1p_mixed(double x) {
    const double y = x * x;
    const double num = 1 + 51064 / 40143 * x + y * (44320 / 120429 + 320 / 40143 * x);
    const double den = 1 + 23712 / 13381 * x + y * (12320 / 13381 + 5120 / 40143 * x);
    return x * num / den;
}
```

Note that the value \( y = x^2 \) can be re-used in the calculation of both the numerator and the denominator. A computation of \( y^2 \) is not necessary. This “mixed” implementation requires 8 floating-point multiplications, 1 floating-point division and 6 additions. Note also that a rational function approximant such as Eq. (6) naturally allows for ILP, as the numerator and denominator can be computed in parallel. This is in particular beneficial for long numerator/denominator polynomials, where the cost of the floating-point division is smaller than the gain by the parallel computation of the terms in the numerator and denominator. In order to further reduce the error and/or the number of terms in the approximant, a more “optimized” minimax rational function approximant may be used instead of a Taylor expansion or Padé approximant when approximating a function over a larger interval.
3 ILP-aware approximant of the real dilogarithm

In the following an ILP-aware implementation of the real dilogarithm with double precision is presented, which allows for the simultaneous execution of multiple floating-point operations. The real dilogarithm is defined as

\[ \text{Li}_2(x) = - \int_0^x \frac{\ln(1-t)}{t} \, dt, \quad x < 1. \]  

(7)

For \(|x| < 1\) the real dilogarithm has the series representation

\[ \text{Li}_2(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^2}. \]  

(8)

Further series representations exist, for example the accelerated series

\[ \text{Li}_2(x) = \sum_{k=0}^{\infty} \frac{B_k}{(k+1)!} \left[ -\ln(1-x) \right]^{k+1}, \]  

(9)

where \(B_k\) are the Bernoulli numbers. A series representation in terms of Chebyshev polynomials of the first kind \(T_n(x)\) is given in Ref. [5],

\[ \text{Li}_2(x) = \sum_{k=0}^{\infty} a_n T_n(2x-1), \]  

(10)

which is used for example in the ROOT library [6]. The r.h.s. of Eqs. (8)–(10) can be summed, for example, using Horner’s scheme or Clenshaw’s algorithm [12], respectively. These summation techniques are, however, purely sequential and thus do not make use of ILP. In the following an approximant of the real dilogarithm is presented, which makes use of ILP, using a rational function approximation in combination with Estrin’s scheme, similar to the approach used in Eq. (6).

We define the real dilogarithm \(\text{Li}_2(x)\) for all \(x \in \mathbb{R}\) as the real part of its complex continuation. The real dilogarithm can be mapped onto the interval \([0, 1/2]\) by using the following identities [1]:

\[ \text{Li}_2(x) = \ln(1-x) \left[ \frac{1}{2} \ln(1-x) - \ln(-x) \right] - \frac{\pi^2}{6}, \]

(11)

\[ + \text{Li}_2 \left( \frac{1}{1-x} \right), \quad x \leq -1, \]

\[ \text{Li}_2(x) = - \text{Li}_2 \left( \frac{x}{x-1} \right) - \frac{1}{2} \ln^2(1-x), \]

(12)

\[ -1 < x < 0, \]

\[ \text{Li}_2(x) = - \text{Li}_2(1-x) + \frac{\pi^2}{6} - \ln(x) \ln(1-x), \]

(13)

\[ \frac{1}{2} < x < 1, \]

\[ 0 < x < 1. \]

Table 1: Coefficients of the numerator and denominator polynomials for the minimax approximant (17).

| Coefficient | Value |
|-------------|-------|
| \(p_0\)     | 0.9999999999999502 \(\times 10^{-6}\) |
| \(p_1\)     | -2.688392681856542340 \(\times 10^{-6}\) |
| \(p_2\)     | 2.647722699473109692 \(\times 10^{-6}\) |
| \(p_3\)     | -1.1538559607887416355 \(\times 10^{-6}\) |
| \(p_4\)     | 2.08860779520607837 \(\times 10^{-6}\) |
| \(p_5\)     | -1.08597713415246084 \(\times 10^{-2}\) |
| \(q_0\)     | 0.00000000000000000 \(\times 10^{1}\) |
| \(q_1\)     | -2.93839268185653458 \(\times 10^{-6}\) |
| \(q_2\)     | 3.27120932930186538 \(\times 10^{-6}\) |
| \(q_3\)     | -1.70767021739542894 \(\times 10^{-6}\) |
| \(q_4\)     | 4.15960172284006383 \(\times 10^{-6}\) |
| \(q_5\)     | -3.98013437540844925 \(\times 10^{-6}\) |
| \(q_6\)     | 8.274366897446659035 \(\times 10^{-4}\) |

The coefficients \(p_k\) and \(q_k\) are listed in Table 1. The approximant on the r.h.s. of Eq. (17) has a maximum relative error of around \(5 \times 10^{-17}\). This error is small enough so that the approximant Eq. (17) can be used for the evaluation of \(\text{Li}_2(x)\) with double precision. Note that the approximant on the r.h.s. of Eq. (17) is very similar to the approximant presented in Ref. [4] (DILOG 0011), although with slightly different coefficients. In order to allow for the use of ILP in the evaluation of the numerator and the denominator on the r.h.s. of Eq. (17) we use Estrin’s scheme and write

\[ \text{Li}_2(x) \approx x \frac{P(x)}{Q(x)}, \quad 0 \leq x \leq \frac{1}{2}, \]  

(18)

with

\[ P(x) = p_0 + p_1 x + (p_2 + p_3 x) y + (p_4 + p_5 x) z, \]

(19)
Table 2: Run-time in seconds for the calculation of \( L_2(x) \) for different implementations on different CPU architectures with different compilers.

| Implementation | i7-4700MQ | i7-5600U |
|----------------|-----------|-----------|
| g++ 9.3.0      | 0.0076    | 0.0058    |
| g++ 10.2.1     | 0.0115    | 0.0085    |
| Cephes [8]      | 0.0136    | 0.0119    |
| Algorithm 327 [2] | 0.0229    | 0.0172    |
| Chebyshev [5, 6] | 0.0718    | 0.0515    |
| Algorithm 490 [3] | 0.1057    | 0.0576    |
| GSL [7]         | 0.2091    | 0.0898    |

For one, Cephes uses a rational function approximation with more terms in the numerator and denominator. Furthermore, Cephes evaluates the numerator and denominator polynomials using Horner’s scheme, which is purely sequential.

Algorithm 327 [2], Algorithm 490 [3] and the implementation found in the GNU Scientific Library (GSL) [7] use series expansions, which are summed using Horner’s scheme. These algorithms thus do not make use of ILP, which is one reason for their longer run-time. Furthermore, Algorithm 490 and most series expansions in the GSL use expensive floating-point divisions inside loops, which may be another reason for the increased run-time.

The representation in terms of Chebyshev polynomials [5] is implemented in the ROOT program library [6]. In this implementation the polynomials are summed using Clenshaw’s algorithm, which is also purely sequential and slightly more complex than Horner’s scheme. This is a reason why the implementation in [6] has a larger run-time than the rational function approximants discussed above.

4 Run-time comparison

In Table 2 the run-time of different C implementations for the real dilogarithm is compared to the implementation given in the appendix on two different CPU architectures. On each architecture the implementations are compiled with g++ with optimization level 02. The shown run-time denotes the total wall clock time for the calculation of \( L_2(x) \) for \( 10^6 \) uniformly distributed random values \( x \in [0, 1/2] \). The choice of this interval ensures that the measurement is only sensitive to the random values \( x \) and \( z = y^2 \). A C implementation of Eq. (18) can be found in the appendix.

Q(x) = g_0 + g_1 x + (g_2 + g_3 x) y + (g_4 + g_5 x + g_6 y) z,  
(20)

where \( y = x^2 \) and \( z = y^2 \). A C implementation of Eq. (18) can be found in the appendix.

5 Summary

In this paper different approaches for the numerical calculation of the real dilogarithm have been compared w.r.t. their potential for the use of instruction-level parallelism (ILP). We found that a rational minimax approximant in combination with Estrin’s scheme to evaluate the numerator/denominator polynomials provides both a sufficient numerical precision and a high degree of ILP, potentially leading to a reduced run-time when executed on an appropriate CPUs. A corresponding approximant and a C implementation have been presented and compared to several existing implementations w.r.t. their run-time. The C implementation of the presented approximant can be found in the appendix. C++, Fortran, Julia and Rust implementations can be found in [14–16, respectively.

A Implementation of the real dilogarithm

```c
#include <math.h>

double li2(double x) {
    const double PI = 3.1415926535897932;
    const double P[] = { 
        0.9999999999999999502e+0, 
        -2.6883926818565423430e+0, 
        2.6477222699473105692e+0, 
        -1.1538559670878416355e+0, 
        2.08860779502067837e+0, 
        -1.0859777134152463084e+2 
    };
    return PI * x - 1.2 * li2(1 - x);
}
```
```c
const double Q[0] = {
    1.000000000000000e+0,
    -2.9383926185656354858e-09,
    3.2712093291018635389e+0,
    -1.1706702173954829421e+0,
    4.15906172284006038361e-1,
    -3.9801343754084842956e-2,
    8.274366897446659035e-4
};

double y = 0, r = 0, s = 1;
if (x < -1) {
    const double l = log(1 - x);
    y = 1 / (1 - x);
    r = -PI*PI/6 + l * (0.5*l - log(-x));
    s = 1;
} else if (x == -1) {
    return -PI*PI/12;
} else if (x < 0) {
    const double l = log1p(-x);
    y = x / (x - 1);
    r = -0.5*l*1;
    s = -1;
} else if (x == 0) {
    return 0;
} else if (x < 0.5) {
    y = x;
    r = 0;
    s = 1;
} else if (x < 1) {
    y = 1 - x;
    r = PI*PI/6 - log(x)*log(y);
    s = -1;
} else if (x == 1) {
    return PI*PI/6;
} else if (x < 2) {
    const double l = log(x);
    y = 1 - 1/x;
    r = PI*PI/6 - 1*(log(y) + 0.5*l*1);
    s = 1;
} else {
    const double l = log(x);
    y = 1/x;
    r = PI*PI/3 - 0.5*l*1;
    s = -1;
}

const double y2 = y*y;
const double y4 = y2*y2;
const double p = P[0] + y*P[1]
    + y2*(P[2] + y*P[3])
    + y4*(P[4] + y*P[5]);
const double q = Q[0] + y*Q[1]
    + y2*(Q[2] + y*Q[3])
    + y4*(Q[4] + y*Q[5] + y2*Q[6]);
return r + s*y*p/q;
```

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