# THE MPFR LIBRARY: ALGORITHMS AND PROOFS

# THE MPFR TEAM

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#### 1. Notations and Assumptions

In the whole document,  $\mathcal{N}()$  denotes rounding to nearest,  $\mathcal{Z}()$  rounding toward zero,  $\triangle()$  rounding toward plus infinity,  $\nabla()$  rounding toward minus infinity, and  $\circ()$  any of those four rounding modes.

In the whole document, except special notice, all variables are assumed to have the same precision, usually denoted p.

#### 2. Error calculus

Let n — the working precision — be a positive integer (considered fixed in the following). We write any nonzero real number x in the form  $x = m \cdot 2^e$  with  $\frac{1}{2} \le |m| < 1$  and e := Exp(x), and we define  $\text{ulp}(x) := 2^{\text{Exp}(x) - n}$ .

### 2.1. Ulp calculus.

**Rule 1.** 
$$2^{-n}|x| < \text{ulp}(x) \le 2^{-n+1}|x|$$
.

*Proof.* Obvious from 
$$x = m \cdot 2^e$$
 with  $\frac{1}{2} \le |m| < 1$ .

**Rule 2.** If a and b have same precision n, and  $|a| \leq |b|$ , then  $ulp(a) \leq ulp(b)$ .

*Proof.* Write 
$$a = m_a \cdot 2^{e_a}$$
 and  $b = m_b \cdot 2^{e_b}$ . Then  $|a| \leq |b|$  implies  $e_a \leq e_b$ , thus  $\text{ulp}(a) = 2^{e_a - n} \leq 2^{e_b - n} = \text{ulp}(b)$ .

**Rule 3.** Let x be a real number, and y = o(x). Then  $|x - y| \le \frac{1}{2}\min(\text{ulp}(x), \text{ulp}(y))$  in rounding to nearest, and  $|x - y| \le \min(\text{ulp}(x), \text{ulp}(y))$  for the other rounding modes.

*Proof.* First consider rounding to nearest. By definition, we have  $|x-y| \leq \frac{1}{2} \text{ulp}(y)$ . If  $\text{ulp}(y) \leq \text{ulp}(x)$ , then  $|x-y| \leq \frac{1}{2} \text{ulp}(y) \leq \frac{1}{2} \text{ulp}(x)$ . The only difficult case is when ulp(x) < ulp(y), but then necessarily y is a power of two; since in that case  $y - \frac{1}{2} \text{ulp}(y)$  is exactly representable, the maximal possible difference between x and y is  $\frac{1}{4} \text{ulp}(y) = \frac{1}{2} \text{ulp}(x)$ , which concludes the proof in the rounding to nearest case.

In rounding to zero, we always have  $\operatorname{ulp}(y) \leq \operatorname{ulp}(x)$ , so the rule holds. In rounding away from zero, the only difficult case is when  $\operatorname{ulp}(x) < \operatorname{ulp}(y)$ , but then y is a power of two, and since  $y - \frac{1}{2}\operatorname{ulp}(y)$  is exactly representable, the maximal possible difference between x and y is  $\frac{1}{2}\operatorname{ulp}(y) = \operatorname{ulp}(x)$ , which concludes the proof.

**Rule 4.**  $\frac{1}{2}|a| \cdot \text{ulp}(b) < \text{ulp}(ab) < 2|a| \cdot \text{ulp}(b)$ .

Proof. Write  $a = m_a 2^{e_a}$ ,  $b = m_b \cdot 2^{e_b}$ , and  $ab = m2^e$  with  $\frac{1}{2} \le m_a$ ,  $m_b$ , m < 1, then  $\frac{1}{4} 2^{e_a + e_b} \le |ab| < 2^{e_a + e_b}$ , thus  $e = e_a + e_b$  or  $e = e_a + e_b - 1$ , which implies  $\frac{1}{2} 2^{e_a} \text{ulp}(b) \le \text{ulp}(ab) \le 2^{e_a} \text{ulp}(b)$  using  $2^{e_b - n} = \text{ulp}(b)$ , and the rule follows from the fact that  $|a| < 2^{e_a} \le 2|a|$  (equality on the right side can occur only if  $e = e_a + e_b$  and  $m_a = \frac{1}{2}$ , which are incompatible).

**Rule 5.**  $ulp(2^k a) = 2^k ulp(a)$ .

*Proof.* Easy: if  $a = m_a \cdot 2^{e_a}$ , then  $2^k a = m_a \cdot 2^{e_a + k}$ .

**Rule 6.** Let x > 0,  $\circ(\cdot)$  be any rounding, and  $u := \circ(x)$ , then  $\frac{1}{2}u < x < 2u$ .

*Proof.* Assume  $x \geq 2u$ , then 2u is another representable number which is closer from x than u, which leads to a contradiction. The same argument proves  $\frac{1}{2}u < x$ .

**Rule 7.**  $\frac{1}{2}|a| \cdot \text{ulp}(1) < \text{ulp}(a) \le |a| \cdot \text{ulp}(1)$ .

*Proof.* The left inequality comes from Rule 4 with b=1, and the right one from  $|a|\text{ulp}(1) \ge \frac{1}{2}2^{e_a}2^{1-n} = \text{ulp}(a)$ .

**Rule 8.** For any  $x \neq 0$  and any rounding mode  $\circ(\cdot)$ , we have  $\operatorname{ulp}(x) \leq \operatorname{ulp}(\circ(x))$ , and equality holds when rounding toward zero, toward  $-\infty$  for x > 0, or toward  $+\infty$  for x < 0.

Proof. Without loss of generality, assume x > 0. Let  $x = m \cdot 2^e$  with  $\frac{1}{2} \le m < 1$ . As  $\frac{1}{2}2^{e_x}$  is a machine number, necessarily  $o(x) \ge \frac{1}{2}2^{e_x}$ , thus by Rule 2, then  $\operatorname{ulp}(o(x)) \ge 2^{e_x-n} = \operatorname{ulp}(x)$ . If we round toward zero, then  $o(x) \le x$  and by Rule 2 again,  $\operatorname{ulp}(o(x)) \le \operatorname{ulp}(x)$ .

Rule 9.

For 
$$\operatorname{error}(u) \le k_u \operatorname{ulp}(u)$$
,  $u.c_u^- \le x \le u.c_u^+$   
with  $c_u^- = 1 - k_u 2^{1-p}$  and  $c_u^+ = 1 + k_u 2^{1-p}$ 

For 
$$u = \circ(x)$$
,  $u.c_u^- \le x \le u.c_u^+$   
if  $u = \triangle(x)$ , then  $c_u^+ = 1$   
if  $u = \nabla(x)$ , then  $c_u^- = 1$   
if for  $x < 0$  and  $u = \mathcal{Z}(x)$ , then  $c_u^+ = 1$   
if for  $x > 0$  and  $u = \mathcal{Z}(x)$ , then  $c_u^- = 1$   
else  $c_u^- = 1 - 2^{1-p}$  and  $c_u^+ = 1 + 2^{1-p}$ 

2.2. Relative error analysis. Another way to get a bound on the error, is to bound the relative error. This is sometimes easier than using the "ulp calculus" especially when performing only multiplications or divisions.

**Rule 10.** If  $u := \circ_p(x)$ , then we can write both:

$$u = x(1 + \theta_1), \qquad x = u(1 + \theta_2),$$

where  $|\theta_i| \leq 2^{-p}$  for rounding to nearest, and  $|\theta_i| < 2^{1-p}$  for directed rounding.

*Proof.* This is a simple consequence of Rule 3. For rounding to nearest, we have  $|u-x| \le \frac{1}{2} \text{ulp}(t)$  for t=u or t=x, hence by Rule 1  $|u-x| \le 2^{-p}$ .

**Rule 11.** Assume  $x_1, \ldots, x_n$  are n floating-point numbers in precision p, and we compute an approximation of their product with the following sequence of operations:  $u_1 = x_1, u_2 = \circ(u_1x_2), \ldots, u_n = \circ(u_{n-1}x_n)$ . If rounding away from zero, the total rounding error is bounded by  $2(n-1)\text{ulp}(u_n)$ .

Proof. We can write  $u_1x_2 = u_2(1-\theta_2), \ldots, u_{n-1}x_n = u_n(1-\theta_n)$ , where  $0 \le \theta_i \le 2^{1-p}$ . We get  $x_1x_2\ldots x_n = u_n(1-\theta_2)\ldots (1-\theta_n)$ , which we can write  $u_n(1-\theta)^{n-1}$  for some  $0 \le \theta \le 2^{1-p}$  by the intermediate value theorem. Since  $1-nt \le (1-t)^n \le 1$ , we get  $|x_1x_2\ldots x_n-u_n| \le (n-1)2^{1-p}|u_n| \le 2(n-1)\text{ulp}(u_n)$  by Rule 1.

2.3. Generic error of addition/subtraction. We want to compute the generic error of the subtraction, the following rules apply to addition too.

Note: 
$$\operatorname{error}(u) \leq k_u \operatorname{ulp}(u)$$
,  $\operatorname{error}(v) \leq k_v \operatorname{ulp}(v)$ 

Note: 
$$\operatorname{ulp}(w) = 2^{e_w - p}$$
,  $\operatorname{ulp}(u) = 2^{e_u - p}$ ,  $\operatorname{ulp}(v) = 2^{e_v - p}$  with  $p$  the precision  $\operatorname{ulp}(u) = 2^{d + e_w - p}$ ,  $\operatorname{ulp}(v) = 2^{d' + e_w - p}$ , with  $d = e_u - e_w$   $d' = e_v - e_w$   $\operatorname{error}(w) \leq c_w \operatorname{ulp}(w) + k_u \operatorname{ulp}(u) + k_v \operatorname{ulp}(v)$   $= (c_w + k_u 2^d + k_v 2^{d'}) \operatorname{ulp}(w)$ 

If  $(u \geq 0 \text{ and } v \geq 0)$  or  $(u \leq 0 \text{ and } v \leq 0)$   $\operatorname{error}(w) \leq (c_w + k_u + k_v) \operatorname{ulp}(w)$ 

Note: If  $w = \mathcal{N}(u + v)$  Then  $c_w = \frac{1}{2}$  else  $c_w = 1$ 

2.4. **Generic error of multiplication.** We want to compute the generic error of the multiplication. We assume here u, v > 0 are approximations of exact values respectively x and y, with  $|u - x| \le k_u \operatorname{ulp}(u)$  and  $|v - y| \le k_v \operatorname{ulp}(v)$ .

$$w = \circ(uv)$$

$$\begin{aligned}
&\text{error}(w) &= |w - xy| \\
&\leq |w - uv| + |uv - xy| \\
&\leq c_w \text{ulp}(w) + \frac{1}{2}[|uv - uy| + |uy - xy| + |uv - xv| + |xv - xy|] \\
&\leq c_w \text{ulp}(w) + \frac{u + x}{2} k_v \text{ulp}(v) + \frac{v + y}{2} k_u \text{ulp}(u) \\
&\leq c_w \text{ulp}(w) + \frac{u(1 + c_u^+)}{2} k_v \text{ulp}(v) + \frac{v(1 + c_v^+)}{2} k_u \text{ulp}(u) \quad \text{[Rule 9]} \\
&\leq c_w \text{ulp}(w) + (1 + c_u^+) k_v \text{ulp}(uv) + (1 + c_v^+) k_u \text{ulp}(uv) \quad \text{[Rule 4]} \\
&\leq [c_w + (1 + c_u^+) k_v + (1 + c_v^+) k_u] \text{ulp}(w) \quad \text{[Rule 8]}
\end{aligned}$$

Note: If 
$$w = \mathcal{N}(uv)$$
 Then  $c_w = \frac{1}{2}$  else  $c_w = 1$ 

2.5. **Generic error of inverse.** We want to compute the generic error of the inverse. We assume u > 0.

$$w = \circ(\frac{1}{u})$$
  
Note:  $\operatorname{error}(u) \le k_u \operatorname{ulp}(u)$ 

$$\operatorname{error}(w) = |w - \frac{1}{x}|$$

$$\leq |w - \frac{1}{u}| + |\frac{1}{u} - \frac{1}{x}|$$

$$\leq c_w \operatorname{ulp}(w) + \frac{1}{ux}|u - x|$$

$$\leq c_w \operatorname{ulp}(w) + \frac{k_u}{ux} \operatorname{ulp}(u)$$

Note: 
$$\frac{u}{c_u} \le x$$
 [Rule 6]  
for  $u = \nabla(x)$ ,  $c_u = 1$  else  $c_u = 2$   
then:  $\frac{1}{x} \le c_u \frac{1}{u}$ 

error(w) 
$$\leq c_w \operatorname{ulp}(w) + c_u \frac{k_u}{u^2} \operatorname{ulp}(u)$$
  
 $\leq c_w \operatorname{ulp}(w) + 2 \cdot c_u \cdot k_u \operatorname{ulp}(\frac{u}{u^2})$  [Rule 4]  
 $\leq [c_w + 2 \cdot c_u \cdot k_u] \cdot \operatorname{ulp}(w)$  [Rule 8]  
Note: If  $w = \mathcal{N}(\frac{1}{u})$  Then  $c_w = \frac{1}{2}$  else  $c_w = 1$ 

2.6. **Generic error of division.** We want to compute the generic error of the division. Without loss of generality, we assume all variables are positive.

nerality, we assume all variables are positive. 
$$w = o(\frac{u}{v})$$
Note:  $\operatorname{error}(u) \leq k_u \operatorname{ulp}(u), \operatorname{error}(v) \leq k_v \operatorname{ulp}(v)$ 

$$\operatorname{error}(w) = |w - \frac{x}{y}|$$

$$\leq |w - \frac{u}{v}| + |\frac{u}{v} - \frac{x}{y}|$$

$$\leq c_w \operatorname{ulp}(w) + \frac{1}{vy}|uy - vx|$$

$$\leq c_w \operatorname{ulp}(w) + \frac{1}{vy}[|uy - xy| + |xy - vx|]$$

$$\leq c_w \operatorname{ulp}(w) + \frac{1}{vy}[yk_u \operatorname{ulp}(u) + xk_v \operatorname{ulp}(v)]$$

$$= c_w \operatorname{ulp}(w) + \frac{k_u}{v} \operatorname{ulp}(u) + \frac{k_v x}{vy} \operatorname{ulp}(v)$$
Note: 
$$\frac{\operatorname{ulp}(u)}{v} \leq 2\operatorname{ulp}(\frac{u}{v}) \quad [\operatorname{Rule } 4]$$

$$2\operatorname{ulp}(\frac{u}{v}) \leq 2\operatorname{ulp}(w) \quad [\operatorname{Rule } 8]$$
Note: 
$$x \leq c_u u \text{ and } \frac{v}{c_v} \leq y \quad [\operatorname{Rule } 6]$$
with for  $u = \Delta(x), c_u = 1 \text{ else } c_u = 2$ 
and for  $v = \nabla(y), c_v = 1 \text{ else } c_v = 2$ 
then: 
$$\frac{x}{y} \leq c_u c_v \frac{u}{v}$$

$$v) \leq c_w \operatorname{ulp}(w) + 2.k_u \operatorname{ulp}(w) + c_u.c_v.\frac{k_v u}{v} \operatorname{ulp}(v)$$

$$\operatorname{error}(w) \leq c_{w}\operatorname{ulp}(w) + 2.k_{u}\operatorname{ulp}(w) + c_{u}.c_{v}.\frac{k_{v}u}{vv}\operatorname{ulp}(v)$$

$$\leq c_{w}\operatorname{ulp}(w) + 2.k_{u}\operatorname{ulp}(w) + 2.c_{u}.c_{v}.k_{v}\operatorname{ulp}(\frac{u.v}{v.v}) \quad [\text{Rule 4}]$$

$$\leq [c_{w} + 2.k_{u} + 2.c_{u}.c_{v}.k_{v}].\operatorname{ulp}(w) \quad [\text{Rule 8}]$$

Note: If 
$$w = \mathcal{N}(\frac{u}{v})$$
 Then  $c_w = \frac{1}{2}$  else  $c_w = 1$ 

Note that we can obtain a slightly different result by writing uy - vx = (uy - uv) + (uv - vx) instead of (uy - xy) + (xy - vx).

Another result can be obtained using a relative error analysis. Assume  $x = u(1 + \theta_u)$  and  $y = v(1 + \theta_v)$ . Then  $|\frac{u}{v} - \frac{x}{y}| \le \frac{1}{vy}|uy - uv| + \frac{1}{vy}|uv - xv| = \frac{u}{y}(|\theta_u| + |\theta_v|)$ . If  $v \le y$  and  $\frac{u}{v} \le w$ , this is bounded by  $w(|\theta_u| + |\theta_v|)$ .

2.7. **Generic error of square root.** We want to compute the generic error of the square root of a floating-point number u, itself an approximation to a real x, with  $|u-x| \leq k_u \text{ulp}(u)$ . If  $v = o(\sqrt{u})$ , then:

$$\operatorname{error}(v) := |v - \sqrt{x}| \leq |v - \sqrt{u}| + |\sqrt{u} - \sqrt{x}|$$

$$\leq c_v \operatorname{ulp}(v) + \frac{1}{\sqrt{u} + \sqrt{x}} |u - x|$$

$$\leq c_v \operatorname{ulp}(v) + \frac{1}{\sqrt{u} + \sqrt{x}} k_u \operatorname{ulp}(u)$$

Since by Rule 9 we have  $u.c_u^- \le x$ , it follows  $\frac{1}{\sqrt{x}+\sqrt{u}} \le \frac{1}{\sqrt{u.(1+\sqrt{c_u^-})}}$ :

$$\operatorname{error}(v) \leq c_{v}\operatorname{ulp}(v) + \frac{1}{\sqrt{u}\cdot(1+\sqrt{c_{u}^{-}})}k_{u}\operatorname{ulp}(u)$$

$$\leq c_{v}\operatorname{ulp}(v) + \frac{2}{1+\sqrt{c_{u}^{-}}}k_{u}\operatorname{ulp}(\sqrt{u}) \quad [\text{Rule 4}]$$

$$\leq (c_{v} + \frac{2k_{u}}{1+\sqrt{c_{u}^{-}}})\operatorname{ulp}(v). \quad [\text{Rule 8}]$$

If u is less than x, we have  $c_u^- = 1$  and we get the simpler formula  $|v - \sqrt{x}| \le (c_v + k_u) \operatorname{ulp}(v)$ .

2.8. **Generic error of the exponential.** We want to compute the generic error of the exponential.

$$v = \circ(e^u)$$
  
Note:  $\operatorname{error}(u) \le k_u \operatorname{ulp}(u)$ 

$$\operatorname{error}(v) = |v - e^{x}|$$

$$\leq |v - e^{u}| + |e^{u} - e^{x}|$$

$$\leq c_{v}\operatorname{ulp}(v) + e^{t}|u - x| \text{ with Rolle's theorem, for } t \in [x, u] \text{ or } t \in [u, x]$$

$$\operatorname{error}(v) \leq c_{v}\operatorname{ulp}(v) + c_{u}^{*}e^{u}k_{u}\operatorname{ulp}(u)$$

$$\leq c_{v}\operatorname{ulp}(v) + 2c_{u}^{*}uk_{u}\operatorname{ulp}(e^{u}) \quad [\text{Rule 4}]$$

$$\leq (c_{v} + 2c_{u}^{*}uk_{u})\operatorname{ulp}(v) \quad [\text{Rule 8}]$$

$$\leq (c_{v} + c_{u}^{*}2^{\operatorname{exp}(u)+1}k_{u})\operatorname{ulp}(v)$$

Note: 
$$u = m_u 2^{e_u}$$
 and  $\operatorname{ulp}(u) = 2^{e_u - p}$  with  $p$  the precision Case  $x \le u$   $c_u^* = 1$ 

Case  $u \le x$ 

$$x \le u + k_u \operatorname{ulp}(u)$$

$$e^x \le e^u e^{k_u \operatorname{ulp}(u)}$$

$$e^x \le e^u e^{k_u 2^{e_u - p}}$$
then  $c_u^* = e^{k_u 2^{\operatorname{exp}(u) - p}}$ 

2.9. Generic error of the logarithm. Assume x and u are positive values, with  $|u-x| \le k_u \operatorname{ulp}(u)$ . We additionally assume  $u \le 4x$ . Let  $v = o(\log u)$ .

error(v) = 
$$|v - \log x| \le |v - \log u| + |\log u - \log x|$$
  
 $\le c_v \text{ulp}(v) + |\log \frac{x}{u}| \le c_v \text{ulp}(v) + 2\frac{|x - u|}{u}$   
 $\le c_v \text{ulp}(v) + \frac{2k_u \text{ulp}(u)}{u} \le c_v \text{ulp}(v) + 2k_u \text{ulp}(1)$  [Rule 7]  
 $\le c_v \text{ulp}(v) + 2k_u 2^{1-e_v} \text{ulp}(v) \le (c_v + k_u 2^{2-e_v}) \text{ulp}(v).$ 

We used at line 2 the inequality  $|\log t| \le 2|t-1|$  which holds for  $t \ge \rho$ , where  $\rho \approx 0.203$  satisfies  $\log \rho = 2(\rho - 1)$ . At line 4,  $e_v$  stands for the exponent of v, i.e,  $v = m \cdot 2^{e_v}$  with  $1/2 \le |m| < 1$ .

2.10. **Ulp calculus vs relative error.** The error in ulp (ulp-error) and the relative error are related as follows.

Let n be the working precision. Consider u = o(x), then the error on u is at most  $\text{ulp}(u) = 2^{\text{Exp}(u)-n} \leq |u| \cdot 2^{1-n}$ , thus the relative error is  $\leq 2^{1-n}$ .

Respectively, if the relative error is  $\leq \delta$ , then the error is at most  $\delta |u| \leq \delta 2^n \text{ulp}(u)$ . (Going from the ulp-error to the relative error and back, we lose a factor of two.)

It is sometimes more convenient to use the relative error instead of the error in ulp (ulperror), in particular when only multiplications or divisions are made. In that case, Higham [11] proposes the following framework: we associate to each variable the cumulated number k of roundings that were made. The *i*th rounding introduces a relative error of  $\delta_i$ , with  $|\delta_i| \leq 2^{1-n}$ , i.e. the computed result is  $1 + \delta_i$  times the exact result. Hence k successive roundings give a error factor of  $(1 + \delta_1)(1 + \delta_2) \cdots (1 + \delta_k)$ , which is between  $(1 - \varepsilon)^k$  and  $(1 + \varepsilon)^k$  with  $\varepsilon = 2^{1-n}$ . In particular, if all roundings are away, the final relative error is at most  $k\varepsilon = k \cdot 2^{1-n}$ , thus at most 2k ulps.

**Lemma 1.** If a value is computed by k successive multiplications or divisions, each with rounding away from zero, and precision n, then the final error is bounded by 2k ulps.

If the rounding are not away from zero, the following lemma is still useful [10]:

**Lemma 2.** Let  $\delta_1, \ldots, \delta_n$  be n real values such that  $|\delta_i| \leq \epsilon$ , for  $n\epsilon < 1$ . Then we can write  $\prod_{i=1}^n (1+\delta_i) = 1+\theta$  with

$$|\theta| \le \frac{n\epsilon}{1 - n\epsilon}.$$

*Proof.* The maximum values of  $\theta$  are obtained when all the  $\delta_i$  are  $\epsilon$ , or all are  $-\epsilon$ , thus it suffices to prove

$$(1+\epsilon)^n \le 1 + \frac{n\epsilon}{1-n\epsilon} = \frac{1}{1-n\epsilon}$$
 and  $(1-\epsilon)^n \ge 1 - \frac{n\epsilon}{1-n\epsilon} = \frac{1-2n\epsilon}{1-n\epsilon}$ .

For the first inequality, we have  $(1+\epsilon)^n = e^{n\log(1+\epsilon)}$ , and since  $\log(1+x) \leq x$ , it follows  $(1+\epsilon)^n \le e^{n\epsilon} = \sum_{k\ge 0} \frac{(n\epsilon)^k}{k!} \le \sum_{k\ge 0} (n\epsilon)^k = \frac{1}{1-n\epsilon}.$  For the second inequality, we first prove by induction that  $(1-\epsilon)^n \ge 1-n\epsilon$  for integer

 $n \ge 0$ . It follows  $(1-\epsilon)^n(1-n\epsilon) \ge (1-n\epsilon)^2 \ge 1-2n\epsilon$ , which concludes the proof.

#### 3. Low Level functions

3.1. The mpfr\_add function.

- 2.  $A \leftarrow B1 + (C1 >> d)$
- 3. q <- compute\_carry (B0, C0, rnd)
- 4. A < -A + q
- 3.2. The mpfr\_cmp2 function. This function computes the exponent shift when subtracting c > 0 from  $b \ge c$ . In other terms, if  $\exp(x) := \lfloor \frac{\log x}{\log 2} \rfloor$ , it returns  $\exp(b) - \exp(b - c)$ .

This function admits the following specification in terms of the binary representation of the mantissa of b and c: if  $b = u10^n r$  and  $c = u01^n s$ , where u is the longest common prefix to b and c, and (r,s) do not start with (0,1), then mpfr\_cmp2(b,c) returns |u|+n if r>s, and |u| + n + 1 otherwise, where |u| is the number of bits of u.

As it is not very efficient to compare b and c bit-per-bit, we propose the following algorithm, which compares b and c word-per-word. Here b[n] represents the nth word from the mantissa of b, starting from the most significant word b[0], which has its most significant bit set. The values c[n] represent the words of c, after a possible shift if the exponent of c is smaller than that of b.

```
n = 0; res = 0;
while (b[n] == c[n])
   n++;
   res += BITS_PER_MP_LIMB;
/* now b[n] > c[n] and the first res bits coincide */
```

```
dif = b[n] - c[n];
while (dif == 1)
   n++;
   dif = (dif << BITS_PER_MP_LIMB) + b[n] - c[n];</pre>
   res += BITS_PER_MP_LIMB;
/* now dif > 1 */
res += BITS_PER_MP_LIMB - number_of_bits(dif);
if (!is_power_of_two(dif))
   return res;
/* otherwise result is res + (low(b) < low(c)) */</pre>
   n++;
while (b[n] == c[n]);
return res + (b[n] < c[n]);
```

3.3. The mpfr\_sub function. The algorithm used is as follows, where w denotes the number of bits per word. We assume that a, b and c denote different variables (if a := b or a := c, we have first to copy b or c), and that the rounding mode is either  $\mathcal{N}$  (nearest),  $\mathcal{Z}$  (toward zero), or  $\infty$  (away from zero).

```
Algorithm mpfr_sub.
```

```
Input: b, c of same sign with b > c > 0, a rounding mode \circ \in \{\mathcal{N}, \mathcal{Z}, \infty\}
Side effect: store in a the value of \circ (b-c)
Output: 0 if \circ (b-c) = b-c, 1 if \circ (b-c) > b-c, and -1 if \circ (b-c) < b-c
\mathtt{an} \leftarrow \big\lceil \tfrac{\mathrm{prec}(a)}{w} \big\rceil, \, \mathtt{bn} \leftarrow \big\lceil \tfrac{\mathrm{prec}(b)}{w} \big\rceil, \, \mathtt{cn} \leftarrow \big\lceil \tfrac{\mathrm{prec}(c)}{w} \big\rceil
cancel \leftarrow mpfr\_cmp2(b, c); \quad diff\_exp \leftarrow Exp(b) - Exp(c)
\mathtt{shift_b} \leftarrow (\mathtt{-cancel}) \bmod w; \quad \mathtt{cancel_b} \leftarrow (\mathtt{cancel} + \mathtt{shift_b})/w
if shift_b > 0 then b[0...bn] \leftarrow mpn\_rshift(b[0...bn-1], shift_b); bn \leftarrow
bn + 1
shift_c \leftarrow (diff\_exp - cancel) \mod w; \quad cancel_c \leftarrow (cancel + shift_c - cancel)
diff_exp)/w
if shift_c > 0 then c[0...cn] \leftarrow mpn\_rshift(c[0...cn-1], shift_c); cn \leftarrow
cn + 1
\exp(a) \leftarrow \exp(b) - \operatorname{cancel}; \quad \operatorname{sign}(a) \leftarrow \operatorname{sign}(b)
a[0...an-1] \leftarrow b[bn-cancel_b-an...bn-cancel_b-1]
a[0...an-1] \leftarrow a[0...an-1] - c[cn-cancel_c-an...cn-cancel_c-1]
\operatorname{sh} \leftarrow \operatorname{an} \cdot w - \operatorname{prec}(a); \quad r \leftarrow a[0] \mod 2^{\operatorname{sh}}; \quad a[0] \leftarrow a[0] - r
if \circ = \mathcal{N} and \mathtt{sh} > 0 then
   if r > 2^{\sinh - 1} then a \leftarrow a + \text{ulp}(a); return 1 elif 0 < r < 2^{\sinh - 1} then return
-1
elif \circ \in \{\mathcal{Z}, \infty\} and r > 0 then
    if \circ = \mathcal{Z} return -1 else a \leftarrow a + \text{ulp}(a); return 1
```

```
\begin{array}{l} \operatorname{bl} \leftarrow \operatorname{bn} - \operatorname{an} - \operatorname{cancel}_{\operatorname{b}} \\ \operatorname{cl} \leftarrow \operatorname{cn} - \operatorname{an} - \operatorname{cancel}_{\operatorname{c}} \\ \text{for } k = 0 \text{ while } \operatorname{bl} > 0 \text{ and } \operatorname{cl} > 0 \text{ do} \\ \operatorname{bl} \leftarrow \operatorname{bl} - 1; \operatorname{bp} \leftarrow b[\operatorname{bl}] \\ \operatorname{cl} \leftarrow \operatorname{cl} - 1; \operatorname{cp} \leftarrow c[\operatorname{cl}] \\ \operatorname{if} \circ = \mathcal{N} \text{ and } k = 0 \text{ and } \operatorname{sh} = 0 \text{ then} \\ \operatorname{if } \operatorname{cp} \geq 2^{w-1} \text{ then } \operatorname{return} - 1 \\ r \leftarrow \operatorname{bp} - \operatorname{cp}; \quad \operatorname{cp} \leftarrow \operatorname{cp} + 2^{w-1} \\ \operatorname{if } \operatorname{bp} < \operatorname{cp } \operatorname{then} \\ \operatorname{if } \circ = \mathcal{Z} \text{ then } a \leftarrow a - \operatorname{ulp}(a); \quad \operatorname{if } \circ = \infty \text{ then } \operatorname{return} 1 \text{ else } \operatorname{return} \\ -1 \quad \operatorname{if } \operatorname{bp} > \operatorname{cp } \operatorname{then} \\ \operatorname{if } \circ = \mathcal{Z} \text{ then } \operatorname{return} - 1 \text{ else } a \leftarrow a + \operatorname{ulp}(a); \operatorname{return} 1 \\ \operatorname{if } \circ = \mathcal{N} \text{ and } r > 0 \text{ then} \\ \operatorname{if } a[0] \operatorname{div} 2^{\operatorname{sh}} \text{ is odd } \operatorname{then} a \leftarrow a + \operatorname{ulp}(a); \operatorname{return} 1 \text{ else } \operatorname{return} - 1 \\ \operatorname{Return} 0. \end{array}
```

where b[i] and c[i] is meant as 0 for negative i, and c[i] is meant as 0 for  $i \ge cn$  (cancel<sub>b</sub>  $\ge 0$ , but cancel<sub>c</sub> may be negative).

3.4. The mpfr\_mul function. mpfr\_mul uses two algorithms: if the precision of the operands is small enough, a plain multiplication using mpn\_mul is used (there is no error, except in the final rounding); otherwise it uses mpfr\_mulhigh\_n.

In this case, it trunks the two operands to m limbs:  $1/2 \le b < 1$  and  $1/2 \le c < 1$ , b = bh + bl and c = ch + cl ( $B = 2^{32}or2^{64}$ ). The error comes from:

- Truncation:  $\leq bl.ch + bh.cl + bl.cl \leq bl + cl \leq 2B^{-m}$
- Mulders: Assuming  $\operatorname{error}(Mulders(n)) \leq \operatorname{error}(mulhigh\_basecase(n))$ ,

error(mulhigh(n)) 
$$\leq (n-1)(B-1)^2 B^{-n-2} + \dots + 1(B-1)^2 B^{-2n}$$
  

$$= \sum_{i=1}^{n-1} (n-i)(B-1)^2 B^{-n-1-i} = (B-1)^2 B^{-n-1} \sum_{i=1}^{n-1} B^{-i}$$

$$= (b-1)^2 B^{-n-1} \frac{B^{1-n} - n + nB - B}{(1-B)^2} \leq nB^{-n}.$$

Total error:  $\leq (m+2)B^{-m}$ .

3.5. The mpfr\_div function. The goals of the code of the mpfr\_div function include the fact that the complexity should, while preserving correct rounding, depend on the precision required on the result rather than on the precision given on the operands.

Let u be the dividend, v the divisor, and p the target precision for the quotient. We denote by q the real quotient u/v, with infinite precision, and  $n \geq p$  the working precision. The idea — as in the square root algorithm below — is to use GMP's integer division: divide the most 2n or 2n-1 significant bits from u by the most n significant bits from v will give a good approximation of the quotient's integer significand. The main difficulties arise when u and v have a larger precision than 2n and n respectively, since we have to truncate them. We distinguish two cases: whether the divisor is truncated or not.

3.5.1. Full divisor. This is the easy case. Write  $u = u_1 + u_0$  where  $u_0$  is the truncated part, and  $v = v_1$ . Without loss of generality we can assume that  $\text{ulp}(u_1) = \text{ulp}(v_1) = 1$ , thus  $u_1$  and  $v_1$  are integers, and  $0 \le u_0 < 1$ . Since  $v_1$  has n significant bits, we have  $2^{n-1} \le v_1 < 2^n$ . (We normalize u so that the integer quotient gives exactly n bits; this is easy by comparing the most significant bits of u and v, thus  $2^{2n-2} \le u_1 < 2^{2n}$ .) The integer division of  $u_1$  by  $v_1$  yields  $q_1$  and r such that  $u_1 = q_1v_1 + r$ , with  $0 \le r < v_1$ , and  $q_1$  having exactly n bits. In that case we have

$$q_1 \le q = \frac{u}{v} < q_1 + 1.$$

Indeed,  $q = \frac{u}{v} \ge \frac{u_1}{v_1} = \frac{q_1 v_1 + r}{v_1}$ , and  $q \le \frac{u_1 + u_0}{v_1} \le q_1 + \frac{r + u_0}{v_1} < q_1 + 1$ , since  $r + u_0 < r + 1 \le v_1$ .

3.5.2. Truncated divisor. This is the hard case. Write  $u = u_1 + u_0$ , and  $v = v_1 + v_0$ , where  $0 \le u_0, v_0 < 1$  with the same conventions as above. We prove in that case that:

(1) 
$$q_1 - 2 < q = \frac{u}{v} < q_1 + 1.$$

The upper bound holds as above. For the lower bound, we have  $u - (q_1 - 2)v > u_1 - (q_1 - 2)(v_1 + 1) \ge q_1v_1 - (q_1 - 2)(v_1 + 1) = 2(v_1 + 1) - q_1 \ge 2^n - q_1 > 0$ . This lower bound is the best possible, since  $q_1 - 1$  would be wrong; indeed, consider n = 3,  $v_1 = 4$ ,  $v_0 = 7/8$ , u = 24: this gives  $q_1 = 6$ , but  $u/v = 64/13 < q_1 - 1 = 5$ .

As a consequence of Eq. (1), if the open interval  $(q_1 - 2, q_1 + 1)$  contains no rounding boundary for the target precision, we can deduce the correct rounding of u/v just from the value of  $q_1$ . In other words, for directed rounding, the two only "bad cases" are when the binary representation of  $q_1$  ends with 0000 or 0001. We even can decide if rounding is correct,

since when  $q_1$  ends with 0010, the exact value cannot end with 0000, and similarly when  $q_1$  ends with 1111. Hence if n = p + k, i.e. if we use k extra bits with respect to the target precision p, the failure probability is  $2^{1-k}$ .

3.5.3. Avoiding Ziv's strategy. In the failure case  $(q_1 \text{ ending with } 000...000x \text{ with directed rounding, or } 100...000x \text{ with rounding to nearest})$ , we could try again with a larger working precision p. However, we then need to perform a second division, and we are not sure this new computation will enable us to conclude. In fact, we can conclude directly. Recall that  $u_1 = q_1v_1 + r$ . Thus  $u = q_1v + (r + u_0 - q_1v_0)$ . We have to decide which of the following five cases holds: (a)  $q_1 - 2 < q < q_1 - 1$ , (b)  $q = q_1 - 1$ , (c)  $q_1 - 1 < q < q_1$ , (d)  $q = q_1$ , (e)  $q_1 < q < q_1 + 1$ .

$$\begin{array}{l} s \leftarrow q_1 v_0 \\ \textbf{if } s < r + u_0 \textbf{ then } q \in (q_1, q_1 + 1) \\ \textbf{elif } s = r + u_0 \textbf{ then } q = q_1 \\ \textbf{else} \\ t \leftarrow s - (r + u_0) \\ \textbf{if } t < v \textbf{ then } q \in (q_1 - 1, q_1) \\ \textbf{elif } t = v \textbf{ then } q = q_1 - 1 \\ \textbf{else } q \in (q_1 - 2, q_1 - 1) \end{array}$$

3.6. The mpfr\_sqrt function. The mpfr\_sqrt implementation uses the mpn\_sqrtrem function from GMP's mpn level: given a positive integer m, it computes s and r such that  $m=s^2+r$  with  $s^2\leq m<(s+1)^2$ , or equivalently  $0\leq r\leq 2s$ . In other words, s is the integer square root of m, rounded toward zero.

The idea is to multiply the input significand by some power of two, in order to obtain an integer significand m whose integer square root s will have exactly p bits, where p is the target precision. This is easy: m should have either 2p or 2p-1 bits. For directed rounding, we then know that the result significand will be either s or s+1, depending on the square root remainder r being zero or not.

Algorithm FPSqrt.

Input:  $x = m \cdot 2^e$ , a target precision p, a rounding mode  $\circ$ 

Output:  $y = \circ_p(\sqrt{x})$ 

If e is odd,  $(m', f) \leftarrow (2m, e - 1)$ , else  $(m', f) \leftarrow (m, e)$ Write  $m' := m_1 2^{2k} + m_0$ ,  $m_1$  having 2p or 2p - 1 bits,  $0 \le m_0 < 2^{2k}$ 

 $(s,r) \leftarrow \operatorname{SqrtRem}(m_1)$ 

If round to zero or down or  $r = m_0 = 0$ , return  $s \cdot 2^{k+f/2}$ 

else return  $(s+1) \cdot 2^{k+f/2}$ .

In case the input has more than 2p or 2p-1 bits, it needs to be truncated, but the crucial point is that truncated part will not overlap with the remainder r from the integer square root, so the *sticky bit* is simply zero when both parts are zero.

For rounding to nearest, the simplest way is to ask p+1 bits for the integer square root — thus m has now 2p+1 or 2p+2 bits. In such a way, we directly get the rounding bit, which is the parity bit of s, and the sticky bit is determined as above. Otherwise, we have to compare the value of the whole remainder, i.e. r plus the possible truncated input, with s+1/4, since  $(s+1/2)^2=s^2+s+1/4$ . Note that equality can occur—i.e. the "nearest even rounding rule" — only when the input has at least 2p+1 bits; in particular it can not happen in the common case when input and output have the same precision.

3.7. The inverse square root. The inverse square root (function mpfr\_rec\_sqrt) is based on Ziv's strategy and the mpfr\_mpn\_rec\_sqrt function, which given a precision p, and an input  $1 \le a < 4$ , returns an approximation x satisfying

$$x - \frac{1}{2} \cdot 2^{-p} \le a^{-1/2} \le x + 2^{-p}$$
.

The mpfr\_mpn\_rec\_sqrt function is based on Newton's iteration and the following lemma, the proof of which can be found in [6]:

**Lemma 3.** Let A, x > 0, and  $x' = x + \frac{x}{2}(1 - Ax^2)$ . Then

$$0 \le A^{-1/2} - x' = \frac{3}{2} \frac{x^3}{\theta^4} (A^{-1/2} - x)^2,$$

for some  $\theta \in (x, A^{-1/2})$ .

We first describe the recursive iteration:

Algorithm ApproximateInverseSquareRoot.

Input:  $1 \le a, A < 4$  and  $1/2 \le x < 1$  with  $x - \frac{1}{2} \cdot 2^{-h} \le a^{-1/2} \le x + 2^{-h}$  Output: X with  $X - \frac{1}{2} \cdot 2^{-n} \le A^{-1/2} \le X + 2^{-n}$ , where  $n \le 2h - 3$ 

$$\begin{array}{ll} r \leftarrow x^2 & [\text{exact}] \\ s \leftarrow Ar & [\text{exact}] \\ t \leftarrow 1-s & [\text{rounded at weight } 2^{-2h} \text{ toward } -\infty] \\ u \leftarrow xt & [\text{exact}] \\ X \leftarrow x + u/2 & [\text{rounded at weight } 2^{-n} \text{ to nearest}] \end{array}$$

**Lemma 4.** If  $h \ge 11$ ,  $0 \le A - a < 2^{-h}$ , then the output X of algorithm ApproximateInverseSquareRoot satisfies

(2) 
$$X - \frac{1}{2} \cdot 2^{-n} \le A^{-1/2} \le X + 2^{-n}.$$

*Proof.* Firstly,  $a \le A < a + 2^{-h}$  yields  $a^{-1/2} - \frac{1}{2} \cdot 2^{-h} \le A^{-1/2} \le a^{-1/2}$ , thus  $x - 2^{-h} \le A^{-1/2} \le x + 2^{-h}$ .

Lemma 3 implies that the value x' that would return Algorithm ApproximateInverseSquareRoot if there was no rounding error satisfies  $0 \le A^{-1/2} - x' = \frac{3}{2} \frac{x^3}{\theta^4} (A^{-1/2} - x)^2$ . Since  $\theta \in (x, A^{-1/2})$ , and  $A^{-1/2} \le x + 2^{-h}$ , we have  $x \le \theta + 2^{-h}$ , which yields  $\frac{x^3}{\theta^3} \le (1 + \frac{2^{-h}}{\theta})^3 \le (1 + 2^{-10})^3 \le 1.003$  since  $\theta \ge 1/2$  and  $h \ge 11$ . Thus  $0 \le A^{-1/2} - x' \le 3.01 \cdot 2^{-2h}$ .

Finally the errors while rounding 1-s and x+u/2 in the algorithm yield  $\frac{1}{2} \cdot 2^{-n} \le x' - X \le \frac{1}{2} \cdot 2^{-n} + \frac{1}{2} \cdot 2^{-2h}$ , thus the final inequality is:

$$\frac{1}{2} \cdot 2^{-n} \le A^{-1/2} - X \le \frac{1}{2} \cdot 2^{-n} + 3.51 \cdot 2^{-2h}.$$

For  $2h \ge n+3$ , we have  $3.51 \cdot 2^{-2h} \le \frac{1}{2} \cdot 2^{-n}$ , which concludes the proof.

The initial approximation is obtained using a bipartite table for h=11. More precisely, we split a 13-bit input  $a=a_1a_0.a_{-1}...a_{-11}$  into three parts of 5, 4 and 4 bits respectively, say  $\alpha, \beta, \gamma$ , and we deduce a 11-bit approximation  $x=0.x_{-1}x_{-2}...x_{-11}$  of the form  $T_1[\alpha, \beta] + T_2[\alpha, \gamma]$ , where both tables have 384 entries each. Those tables satisfy:

$$x + (\frac{1}{4} - \varepsilon)2^{-11} \le a^{-1/2} \le x + (\frac{1}{4} + \varepsilon)2^{-11},$$

with  $\varepsilon \leq 1.061$ . Note that this does not fulfill the initial condition of Algorithm ApproximateInverseSquareRoot, since we have  $x - 0.811 \cdot 2^{-h} \leq a^{-1/2} \leq x + 1.311 \cdot 2^{-h}$ , which yields  $X - \frac{1}{2} \cdot 2^{-n} \leq A^{-1/2} \leq X + 1.21 \cdot 2^{-n}$ , thus the right bound is not a priori fulfilled. However the only problematic case is n = 19, which gives exactly (n+3)/2 = 11, since for  $12 \leq n \leq 18$ , the error terms in  $2^{-2h}$  are halved. An exhaustive search of all possible inputs for h = 11 and n = 19 gives

$$X - \frac{1}{2} \cdot 2^{-n} \le A^{-1/2} \le X + 0.998 \cdot 2^{-n},$$

the worst case being A = 1990149, X = 269098 (scaled by  $2^{19}$ ). Thus as soon as  $n \ge 2$ , Eq. (2) is fulfilled.

In summary, Algorithm ApproximateInverseSquareRoot provides an approximation X of  $A^{-1/2}$  with an error of at most one ulp. However if the input A was itself truncated at precision  $\geq p$  from an input  $A_0$  — for example when the output precision p is less than the input precision — then we have  $|X-A^{-1/2}| \leq \text{ulp}(X)$ , and  $|A^{-1/2}-A_0^{-1/2}| \leq \frac{1}{2}|A-A_0|A^{-3/2} \leq \frac{1}{2}\frac{|A-A_0|}{A}A^{-1/2} \leq 2^{-p}A^{-1/2} \leq \text{ulp}(X)$ , thus  $|X-A_0^{-1/2}| \leq 2 \text{ulp}(X)$ .

3.8. The mpfr\_remainder and mpfr\_remquo functions. The mpfr\_remainder and mpfr\_remquo are useful functions for argument reduction. Given two floating-point numbers x and y, mpfr\_remainder computes the correct rounding of  $x \operatorname{cmod} y := x - qy$ , where  $q = \lfloor x/y \rfloor$ , with ties rounded to the nearest even integer, as in the rounding to nearest mode.

Additionally, mpfr\_remquo returns a value congruent to q modulo  $2^n$ , where n is a small integer (say  $n \leq 64$ , see the documentation), and having the same sign as q or being zero. This can be efficiently implemented by calling mpfr\_remainder on x and  $2^ny$ . Indeed, if  $x = r' \operatorname{cmod}(2^ny)$ , and r' = q'y + r with  $|r| \leq y/2$ , then  $q \equiv q' \mod 2^n$ . No double-rounding problem can occur, since if  $x/(2^ny) \in \mathbb{Z} + 1/2$ , then  $r' = \pm 2^{n-1}y$ , thus  $q' = \pm 2^{n-1}$  and r = 0.

Whatever the input x and y, it should be noted that if  $\operatorname{ulp}(x) \geq \operatorname{ulp}(y)$ , then x - qy is always exactly representable in the precision of y unless its exponent is smaller than the minimum exponent. To see this, let  $\operatorname{ulp}(y) = 2^{-k}$ ; multiplying x and y by  $2^k$  we get  $X = 2^k x$  and  $Y = 2^k y$  such that  $\operatorname{ulp}(Y) = 1$ , and  $\operatorname{ulp}(X) \geq \operatorname{ulp}(Y)$ , thus both X and Y are integers. Now perform the division of X by Y, with quotient rounded to nearest: X = qY + R, with  $|R| \leq Y/2$ . Since R is an integer, it is necessarily representable with the precision of Y, and thus of Y. The quotient Y0 of Y1 is the same as that of X2, the remainder X3 is X4.

We assume without loss of generality that x, y > 0, and that ulp(y) = 1, i.e., y is an integer.

```
Algorithm Remainder.
```

Input: x, y with ulp(y) = 1, a rounding mode  $\circ$ 

Output:  $x \operatorname{cmod} y$ , rounded according to  $\circ$ 

1. If ulp(x) < 1, decompose x into  $x_h + x_l$  with  $ulp(x_h) \ge 1$  and  $0 \le x_l < 1$ .

1a.  $r \leftarrow \text{Remainder}(x_h, y) \text{ [exact, } -y/2 \leq r \leq y/2]$ 

1b. if r < y/2 or  $x_l = 0$  then return  $\circ (r + x_l)$ 

1c. else return  $\circ (r + x_l - y) = \circ (x_l - r)$ 

2. Write  $x = m \cdot 2^k$  with k > 0

3.  $z \leftarrow 2^k \mod y$  [binary exponentiation]

4. Return  $\circ (mz \operatorname{cmod} y)$ .

Note: at step (1a) the auxiliary variable r has the precision of y; since  $x_h$  and y are integers, so is r and the result is exact by the above reasoning. At step (1c) we have r = y/2, thus r - y simplifies to -r.

#### 4. High level functions

4.1. The cosine function. To evaluate  $\cos x$  with a target precision of n bits, we use the following algorithm with working precision m, after an additive argument reduction which reduces x in the interval  $[-\pi, \pi]$ , using the mpfr\_remainder function:

$$k \leftarrow \lfloor \sqrt{n/2} \rfloor$$
  
 $r \leftarrow x^2$  rounded up  
 $r \leftarrow r/2^{2k}$   
 $s \leftarrow 1, t \leftarrow 1$   
**for**  $l$  **from** 1 **while**  $\exp(t) \ge -m$   
 $t \leftarrow t \cdot r$  rounded up  
 $t \leftarrow \frac{t}{(2l-1)(2l)}$  rounded up  
 $s \leftarrow s + (-1)^l t$  rounded down

do 
$$k$$
 times  
 $s \leftarrow 2s^2$  rounded up  
 $s \leftarrow s - 1$   
return  $s$ 

The error on r after  $r \leftarrow x^2$  is at most  $\mathrm{1ulp}(r)$  and remains  $\mathrm{1ulp}(r)$  after  $r \leftarrow r/2^{2k}$  since that division is just an exponent shift. By induction, the error on t after step l of the for-loop is at most 3lulp(t). Hence as long as 3lulp(t) remains less than  $\leq 2^{-m}$  during that loop (this is possible as soon as  $r < 1/\sqrt{2}$ ) and the loop goes to  $l_0$ , the error on s after the for-loop is at most  $2l_0 2^{-m}$  (for |r| < 1, it is easy to check that s will remain in the interval  $[\frac{1}{2}, 1]$ , thus  $\operatorname{ulp}(s) = 2^{-m}$ ). (An additional  $2^{-m}$  term represents the truncation error, but for  $\tilde{l} = 1$  the value of t is exact, giving  $(2l_0 - 1) + 1 = 2l_0$ .)

Denoting by  $\epsilon_i$  the maximal error on s after the ith step in the do-loop, we have  $\epsilon_0 = 2l_0 2^{-m}$ and  $\epsilon_{k+1} \le 4\epsilon_k + 2^{-m}$ , giving  $\epsilon_k \le (2l_0 + 1/3)2^{2k-m}$ .

4.2. The sine function. The sine function is computed from the cosine, with a working precision of m bits, after an additive argument reduction in  $[-\pi, \pi]$ :

 $c \leftarrow \cos x$  rounded away

 $t \leftarrow c^2$  rounded away

 $u \leftarrow 1 - t$  rounded to zero

 $s \leftarrow \operatorname{sign}(x)\sqrt{u}$  rounded to zero

This algorithm ensures that the approximation s is between zero and  $\sin x$ .

Since all variables are in [-1,1], where ulp()  $\leq 2^{-m}$ , all absolute errors are less than  $2^{-m}$ . We denote by  $\epsilon_i$  a generic error with  $0 \le \epsilon_i < 2^{-m}$ . We have  $c = \cos x + \epsilon_1$ ;  $t = c^2 + \epsilon_2 = \cos^2 x + 4\epsilon_3$ ;  $u = 1 - t - \epsilon_4 = 1 - \cos^2 x - 5\epsilon_5$ ;  $|s| = \sqrt{u} - \epsilon_6 = \sqrt{1 - \cos^2 x - 5\epsilon_5} - \epsilon_6 \ge |\sin x| - \frac{5\epsilon_5}{2|s|} + \epsilon_6$  (by Rolle's theorem,  $|\sqrt{u} - \sqrt{u'}| \le \frac{1}{2\sqrt{v}}|u - u'|$  for  $v \in [u, u']$ , we apply it here with  $u = 1 - \cos^2 x - 5\epsilon_5$ ,  $u' = 1 - \cos^2 x$ .)

Therefore, if  $2^{e-1} \leq |s| < 2^e$ , the absolute error on s is bounded by  $2^{-m}(\frac{5}{2}2^{1-e}+1) \leq$  $2^{3-m-e}$ .

4.2.1. An asymptotically fast algorithm for sin and cos. We extend here the algorithm proposed by Brent for the exponential function to the simultaneous computation of sin and cos. The idea is the following. We first reduce the input x to the range 0 < x < 1/2. Then we decompose x as follows:

$$x = \sum_{i=1}^{k} \frac{r_i}{2^{2^i}},$$

where  $r_i$  is an integer,  $0 \le r_i < 2^{2^{i-1}}$ . We define  $x_j = \sum_{i=j}^k \frac{r_i}{2^{2^i}}$ ; then  $x = x_1$ , and we can write  $x_j = \frac{r_j}{2^{2^j}} + x_{j+1}$ . Thus with  $S_j := \sin \frac{r_j}{2^{2^j}}$  and  $C_j := \cos \frac{r_j}{2^{2^j}}$ :

$$\sin x_j = S_j \cos x_{j+1} + C_j \sin x_{j+1}, \quad \cos x_j = C_j \cos x_{j+1} - S_j \sin x_{j+1}.$$

The 2k values  $S_j$  and  $C_j$  can be computed by a binary splitting algorithm, each one in  $O(M(n)\log n)$ . Then each pair  $(\sin x_j,\cos x_j)$  can be computed from  $(\sin x_{j+1},\sin x_{j+1})$  with four multiplies and two additions or subtractions.

Error analysis. We use here Higham's method. We assume that the values of  $S_j$  and  $C_j$  are approximated up to a multiplicative factor of the form  $(1+u)^3$ , where  $|u| \leq 2^{-p}$ ,  $p \geq 4$  being the working precision. We also assume that  $\cos x_{j+1}$  and  $\sin x_{j+1}$  are approximated with a factor of the form  $(1+u)^{k_j}$ . With rounding to nearest, the values of  $S_j \cos x_{j+1}$ ,  $C_j \sin x_{j+1}$ ,  $C_j \cos x_{j+1}$  and  $S_j \sin x_{j+1}$  are thus approximated with a factor  $(1+u)^{k_j+4}$ . The value of  $\sin x_j$  is approximated with a factor  $(1+u)^{k_j+5}$  since there all terms are nonnegative.

We now analyze the effect of the cancellation in  $C_j \cos x_{j+1} - S_j \sin x_{j+1}$ . We have  $\frac{r_j}{2^{2^j}} < 2^{-2^{j-1}}$ , and for simplicity we define  $l := 2^{j-1}$ ; thus  $0 \le S_j \le 2^{-l}$ , and  $1 - 2^{-2l-1} \le C_j \le 1$ . Similarly we have  $x_{j+1} < 2^{-2l}$ , thus  $0 \le \sin x_{j+1} \le 2^{-2l}$ , and  $1 - 2^{-4l-1} \le \cos x_{j+1} \le 1$ . The error is multiplied by a maximal ratio of

$$\frac{C_j \cos x_{j+1} + S_j \sin x_{j+1}}{C_j \cos x_{j+1} - S_j \sin x_{j+1}} \le \frac{1 + 2^{-l} \cdot 2^{-2l}}{(1 - 2^{-2l-1})(1 - 2^{-4l-1}) - 2^{-l} \cdot 2^{-2l}},$$

which we can bound by

$$\frac{1+2^{-3l}}{1-2^{-2l}} \le \frac{1}{(1-2^{-2l})(1-2^{-3l})} \le \frac{1}{1-2^{-2l+1}}.$$

The product of all those factors for  $j \geq 1$  is bounded by 3 (remember  $l := 2^{j-1}$ ).

In summary, the maximal error is of the form  $3[(1+u)^{5k}-1]$ , where  $2^{2^{k-1}} . For <math>p \ge 4$ ,  $5k \cdot 2^{-p}$  is bounded by 5/16, and  $(1+2^{-p})^{5k}-1 \le e^{5k\cdot 2^{-p}}-1 \le \frac{6}{5} \cdot 5k \cdot 2^{-p} = 6k \cdot 2^{-p}$ . Thus the final relative error bound is  $18k \cdot 2^{-p}$ . Since  $k \le 6$  for  $p \le 2^{64}$ , this gives a uniform relative error bound of  $2^{-p+7}$ .

4.3. The tangent function. The tangent function is computed from the  $mpfr\_sin\_cos$  function, which computes simultaneously sin x and cos x with a working precision of m bits:

$$s, c \leftarrow \circ(\sin x), \circ(\cos x)$$
 [to nearest]  $t \leftarrow \circ(s/c)$  [to nearest]

We have  $s = \sin(x)(1+\theta_1)$  and  $c = \cos(x)(1+\theta_2)$  with  $|\theta_1|, |\theta_2| \le 2^{-m}$ , thus  $t = (\tan x)(1+\theta)^3$  with  $|\theta| \le 2^{-m}$ . For  $m \ge 2$ ,  $|\theta| \le 1/4$ ,  $|(1+\theta)^3 - 1| \le 4|\theta|$ , thus we can write  $t = (\tan x)(1+4\theta)$ , thus  $|t - \tan x| \le 4\text{ulp}(t)$ .

4.4. The exponential function. The mpfr\_exp function implements three different algorithms. For very large precision, it uses a  $\mathcal{O}(M(n)\log^2 n)$  algorithm based on binary splitting (see [13]). This algorithm is used only for precision greater than for example 10000 bits on an Athlon.

For smaller precisions, it uses Brent's method; if  $r = (x - n \log 2)/2^k$  where  $0 \le r < \log 2$ , then

$$\exp(x) = 2^n \cdot \exp(r)^{2^k}$$

and  $\exp(r)$  is computed using the Taylor expansion:

$$\exp(r) = 1 + r + \frac{r^2}{2!} + \frac{r^3}{3!} + \cdots$$

As  $r < 2^{-k}$ , if the target precision is n bits, then only about l = n/k terms of the Taylor expansion are needed. This method thus requires the evaluation of the Taylor series to order n/k, and k squares to compute  $\exp(r)^{2^k}$ . If the Taylor series is evaluated using a naive way,

the optimal value of k is about  $n^{1/2}$ , giving a complexity of  $\mathcal{O}(n^{1/2}M(n))$ . This is what is implemented in mpfr\_exp2\_aux.

If we use a baby step/giant step approach, the Taylor series can be evaluated in  $\mathcal{O}(l^{1/2})$  nonscalar multiplications — i.e., with both operands of full n-bit size — as described in [15], thus the evaluation requires  $(n/k)^{1/2} + k$  multiplications, and the optimal k is now about  $n^{1/3}$ , giving a total complexity of  $\mathcal{O}(n^{1/3}M(n))$ . This is implemented in the function mpfr\_exp2\_aux2. (Note: the algorithm from Paterson and Stockmeyer was rediscovered by Smith, who named it "concurrent series" in [20].)

4.5. The error function. Let n be the target precision, and x be the input value. For  $|x| \ge \sqrt{n \log 2}$ , we have  $|\operatorname{erf} x| = 1$  or  $1^-$  according to the rounding mode. Otherwise we use the Taylor expansion.

#### 4.5.1. Taylor expansion.

erf 
$$z = \frac{2}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(2k+1)} z^{2k+1}$$

erf\_0(z,n), assumes  $z^2 \le n/e$ working precision is m  $y \leftarrow \circ(z^2)$  [rounded up]  $s \leftarrow 1$   $t \leftarrow 1$ for k from 1 do  $t \leftarrow \circ(yt)$  [rounded up]  $t \leftarrow \circ(t/k)$  [rounded up]  $u \leftarrow \circ(\frac{t}{2k+1})$  [rounded up]  $s \leftarrow \circ(s+(-1)^k u)$  [nearest] if  $\exp(u) < \exp(s) - m$  and  $k \ge z^2$  then break  $t \leftarrow 2 \circ (zs)$  [rounded up]  $t \leftarrow \circ(\sqrt{p})$  [rounded down]  $t \leftarrow \circ(t/p)$  [rounded down]  $t \leftarrow \circ(\sqrt{p})$  [rounded down]

Let  $\varepsilon_k$  be the ulp-error on t (denoted  $t_k$ ) after the loop with index k. According to Lemma 1, since  $t_k$  is computed after 2k roundings ( $t_0 = 1$  is exact), we have  $\varepsilon_k \leq 4k$ .

The error on u at loop k is thus at most  $1 + 2\varepsilon_k \le 1 + 8k$ .

Let  $\sigma_k$  and  $\nu_k$  be the exponent shifts between the new value of s at step k and respectively the old value of s, and u. Writing  $s_k$  and  $u_k$  for the values of s and u at the end of step k, we have  $\sigma_k := \exp(s_{k-1}) - \exp(s_k)$  and  $\nu_k := \exp(u_k) - \exp(s_k)$ . The ulp-error  $\tau_k$  on  $s_k$  satisfies  $\tau_k \leq \frac{1}{2} + \tau_{k-1} 2^{\sigma_k} + (1+8k)2^{\nu_k}$ .

The halting condition  $k \geq z^2$  ensures that  $u_j \leq u_{j-1}$  for  $j \geq k$ , thus the series  $\sum_{j=k}^{\infty} u_j$  is an alternating series, and the truncated part is bounded by its first term  $|u_k| < \text{ulp}(s_k)$ . So the ulp-error between  $s_k$  and  $\sum_{k=0}^{\infty} \frac{(-1)^k z^2}{k!(2k+1)}$  is bounded by  $1 + \tau_k$ .

Now the error after  $r \leftarrow 2 \circ (zs)$  is bounded by  $1 + 2(1 + \tau_k) = 2\tau_k + 3$ . That on p after  $p \leftarrow \circ(\pi)$  is 1 ulp, and after  $p \leftarrow \circ(\sqrt{p})$  we get 2 ulps (since  $p \leftarrow \circ(\pi)$  was rounded down).

The final error on r is thus at most  $1 + 2(2\tau_k + 3) + 4 = 4\tau_k + 11$  (since r is rounded up and p is rounded down).

4.5.2. Very large arguments. Since erfc  $x \leq \frac{1}{\sqrt{\pi}xe^{x^2}}$ , we have for  $x^2 \geq n \log 2$  (which implies  $x \ge 1$ ) that erfc  $x \le 2^{-n}$ , thus erf x = 1 or erf  $x = 1 - 2^{-n}$  according to the rounding mode. More precisely, [1, formulæ 7.1.23 and 7.1.24] gives:

$$\sqrt{\pi} x e^{x^2} \operatorname{erfc} x \approx 1 + \sum_{k=1}^n (-1)^k \frac{1 \times 3 \times \dots \times (2k-1)}{(2x^2)^k},$$

with the error bounded in absolute value by the next term and of the same sign.

4.6. The hyperbolic cosine function. The mpfr\_cosh  $(\cosh x)$  function implements the hyperbolic cosine as:

$$\cosh x = \frac{1}{2} \left( e^x + \frac{1}{e^x} \right).$$

The algorithm used for the calculation of the hyperbolic cosine is as follows<sup>1</sup>:

$$\begin{array}{ccc}
u & \leftarrow & \circ(e^x) \\
v & \leftarrow & \circ(u^{-1})
\end{array}$$

$$(4) w \leftarrow \circ (u+v)$$

$$(5) s \leftarrow \frac{1}{2}w$$

(6)

Now, we have to bound the rounding error for each step of this algorithm. First, let us consider the parity of hyperbolic cosine  $(\cosh(-x) = \cosh(x))$ : the problem is reduced to calculate  $\cosh x$  with  $x \ge 0$ . We can deduce  $e^x \ge 1$  and  $0 \le e^{-x} \le 1$ .

 $<sup>^{1}\</sup>circ()$  represent the rounding error and error(u) the error associate with the calculation of u

$$\begin{array}{c} \operatorname{error}(u) \\ u \leftarrow \circ(e^x) \\ -\infty \quad (\bullet) \end{array} \\ |u - e^x| & \leq \operatorname{ulp}(u) \\ |v - e^{-x}| & \text{with } \frac{1}{e^x} \leq \frac{1}{u}, \\ \text{for that we must have } u \leq e^x, \\ \text{it is possible with a rounding of } u \text{ to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{ti is possible with a rounding of } u \text{ to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{ti is possible with a rounding of } u \text{ to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{-x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e^{x}| & \text{to } -\infty \quad (\bullet) \\ |v - e$$

That shows the rounding error on the calculation of  $\cosh x$  can be bound by 5—ulp on the result. So, to calculate the size of intermediary variables, we have to add, at least,  $\lceil \log_2 5 \rceil = 3$  bits the wanted precision.

4.7. The inverse hyperbolic cosine function. The mpfr\_acosh function implements the inverse hyperbolic cosine. For x < 1, it returns NaN; for x = 1, acosh x = 0; for x > 1, the formula acosh  $x = \log(\sqrt{x^2 - 1} + x)$  is implemented using the following algorithm:

$$q \leftarrow \circ(x^2)$$
 [down]  
 $r \leftarrow \circ(q-1)$  [down]  
 $s \leftarrow \circ(\sqrt{r})$  [nearest]  
 $t \leftarrow \circ(s+x)$  [nearest]  
 $u \leftarrow \circ(\log t)$  [nearest]

Let us first assume that  $r \neq 0$ . The error on q is at most  $1 \operatorname{ulp}(q)$ , thus that on r is at most  $\operatorname{ulp}(r) + \operatorname{ulp}(q) = (1+E) \operatorname{ulp}(r)$  with  $d = \operatorname{Exp}(q) - \operatorname{Exp}(r)$  and  $E = 2^d$ . Since r is smaller than

 $x^2-1$ , we can use the simpler formula for the error on the square root, which gives a bound  $(\frac{3}{2}+E)\operatorname{ulp}(s)$  for the error on s, and  $(2+E)\operatorname{ulp}(t)$  for that on t. This gives a final bound of  $(\frac{1}{2}+(2+E)2^{2-\operatorname{Exp}(u)})\operatorname{ulp}(u)$  for the error on u (§2.9). We have:  $2+E \leq 2^{1+\max(1,d)}$ . Thus the rounding error on the calculation of  $\operatorname{acosh} x$  can be bounded by  $(\frac{1}{2}+2^{3+\max(1,d)-\operatorname{Exp}(u)})\operatorname{ulp}(u)$ .

If we obtain r = 0, which means that x is near from 1, we need another algorithm. One has x = 1 + z, with  $0 < z < 2^{-p}$ , where p is the intermediate precision (which may be smaller than the precision of x). The formula can be rewritten:  $a\cosh x = \log(1 + \sqrt{z(2+z)} + z) = \sqrt{2z}(1-\varepsilon(z))$  where  $0 < \varepsilon(z) < z/12$ . We use the following algorithm:

$$q \leftarrow \circ(x-1) \text{ [down]}$$
  
 $r \leftarrow 2q$   
 $s \leftarrow \circ(\sqrt{r}) \text{ [nearest]}$ 

The error on q is at most  $1\operatorname{ulp}(q)$ , thus the error on r is at most  $1\operatorname{ulp}(r)$ . Since r is smaller than 2z, we can use the simpler formula for the error on the square root, which gives a bound  $\frac{3}{2}\operatorname{ulp}(s)$  for the error on s. The error on  $\operatorname{acosh} x$  is bounded by the sum of the error bound on  $\sqrt{2z}$  and  $\varepsilon(z)\sqrt{2z}<\frac{2^{-p}}{12}2^{1+\operatorname{Exp}(s)}=\frac{1}{6}\operatorname{ulp}(s)$ . Thus the rounding error on the calculation of  $\operatorname{acosh} x$  can be bounded by  $\left(\frac{3}{2}+\frac{1}{6}\right)\operatorname{ulp}(s)<2\operatorname{ulp}(s)$ .

4.8. The hyperbolic sine function. The mpfr\_sinh  $(\sinh x)$  function implements the hyperbolic sine as:

$$\sinh x = \frac{1}{2} \left( e^x - \frac{1}{e^x} \right).$$

The algorithm used for the calculation of the hyperbolic sine is as follows<sup>2</sup>:

$$u \leftarrow \circ(e^{x})$$

$$v \leftarrow \circ(u^{-1})$$

$$w \leftarrow \circ(u - v)$$

$$s \leftarrow \frac{1}{2}w$$

Now, we have to bound the rounding error for each step of this algorithm. First, let consider the parity of hyperbolic sine  $(\sinh(-x) = -\sinh(x))$ : the problem is reduced to calculate  $\sinh x$  with  $x \ge 0$ . We can deduce  $e^x \ge 1$  and  $0 \le e^{-x} \le 1$ .

 $<sup>^{2}\</sup>circ()$  represent the rounding error and error(u) the error associated with the calculation of u

That show the rounding error on the calculation of  $\sinh x$  can be bound by  $(1+4\cdot 2^{\exp(u)-\exp(w)})\operatorname{ulp}(w)$ , then the number of bits need to add to the want accuracy to define intermediary variable is :

$$N_t = \lceil \log_2(1 + 4 \cdot 2^{\exp(u) - \exp(w)}) \rceil$$

4.9. The inverse hyperbolic sine function. The  $mpfr_asinh$  (asinhx) function implements the inverse hyperbolic sine as:

$$asinh = \log\left(\sqrt{x^2 + 1} + x\right).$$

The algorithm used for the calculation of the inverse hyperbolic sine is as follows

$$s \leftarrow \circ(x^2)$$

$$t \leftarrow \circ(s+1)$$

$$u \leftarrow \circ(\sqrt{t})$$

$$v \leftarrow \circ(u+x)$$

$$w \leftarrow \circ(\log v)$$

Now, we have to bound the rounding error for each step of this algorithm. First, let consider the parity of hyperbolic arc sine  $(a\sinh(-x) = -a\sinh(x))$ : the problem is reduced to calculate  $a\sinh x$  with  $x \ge 0$ .

error(s) 
$$|s-x^2|$$
  
 $s \leftarrow \circ(x^2)$   $\leq \text{ulp}(s) \ (\star)$   
error(t)  $|t-(x^2+1)|$   $(\star)$  see subsection 2.3  
error(u)  $|u-\sqrt{x^2+1}|$  see subsection 2.7  
 $u \leftarrow \circ(\sqrt{t})$   $\leq 3\text{ulp}(u) \ (\star)$  with  $(\bullet)$   
error(v)  $|v-(\sqrt{x^2+1}+x)|$   $(\star)$  see subsection 2.3  
error(w)  $|v-(\sqrt{x^2+1}+x)|$   $(\star)$  see subsection 2.3  
error(w)  $|w-\log(\sqrt{x^2+1}+x)|$   $(\star)$  see subsection 2.3  
error(w)  $|w-\log(\sqrt{x^2+1}+x)|$   $(\star)$  see subsection 2.9

That shows the rounding error on the calculation of asinhx can be bound by  $(1 + 5.2^{2-\text{Exp}(w)})$  ulp on the result. So, to calculate the size of intermediary variables, we have to add, at least,  $\lceil \log_2(1 + 5.2^{2-\text{Exp}(w)}) \rceil$  bits the wanted precision.

4.10. The hyperbolic tangent function. The hyperbolic tangent (mpfr\_tanh) is computed from the exponential:

$$\tanh x = \frac{e^{2x} - 1}{e^{2x} + 1}.$$

The algorithm used is as follows, with working precision p and rounding to nearest:

$$u \leftarrow \circ(2x)$$

$$v \leftarrow \circ(e^{u})$$

$$w \leftarrow \circ(v+1)$$

$$r \leftarrow \circ(v-1)$$

$$s \leftarrow \circ(r/w)$$

Now, we have to bound the rounding error for each step of this algorithm. First, thanks to the parity of hyperbolic tangent —  $\tanh(-x) = -\tanh(x)$  — we can consider without loss of generality that  $x \ge 0$ .

We use Higham's notation, with  $\theta_i$  denoting variables such that  $|\theta_i| \leq 2^{-p}$ . Firstly, u is exact. Then  $v = e^{2x}(1 + \theta_1)$  and  $w = (e^{2x} + 1)(1 + \theta_2)^2$ . The error on r is bounded by  $\frac{1}{2}\text{ulp}(v) + \frac{1}{2}\text{ulp}(r)$ . Assume  $\text{ulp}(v) = 2^e \text{ulp}(r)$ , with  $e \geq 0$ ; then the error on r is bounded by  $\frac{1}{2}(2^e + 1)\text{ulp}(r)$ . We can thus write  $r = (e^{2x} - 1)(1 + \theta_3)^{2^e + 1}$ , and then  $s = \tanh(x)(1 + \theta_4)^{2^e + 4}$ .

**Lemma 5.** For  $|x| \le 1/2$ , and  $|y| \le |x|^{-1/2}$ , we have:

$$|(1+x)^y - 1| \le 2|y|x.$$

Proof. We have  $(1+x)^y = e^{y\log(1+x)}$ , with  $|y\log(1+x)| \le |x|^{-1/2}|\log(1+x)|$ . The function  $|x|^{-1/2}\log(1+x)$  is increasing on [-1/2,1/2], and takes as values  $\approx -0.490$  in x=-1/2 and  $\approx 0.286$  in x=1/2, thus is bounded in absolute value by 1/2. This yields  $|y\log(1+x)| \le 1/2$ . Now it is easy to see that for  $|t| \le 1/2$ , we have  $|e^t-1| \le 1.3|t|$ . Thus  $|(1+x)^y-1| \le 1.3|y||\log(1+x)|$ . The result follows from  $|\log(1+x)| \le 1.4|x|$  for  $|x| \le 1/2$ , and  $1.3 \times 1.4 \le 2$ .

Applying the above lemma for  $x = \theta_4$  and  $y = 2^e + 4$ , assuming  $2^e + 4 \le 2^{p/2}$ , we get  $s = \tanh(x)[1+2(2^e+4)\theta_5]$ . Since  $2^e+4 \le 2^{\max(3,e+1)}$ , the relative error on s is thus bounded by  $2^{\max(4,e+2)-p}$ .

4.11. The inverse hyperbolic tangent function. The mpfr\_atanh (atanhx) function implements the inverse hyperbolic tangent as:

$$atanh = \frac{1}{2}\log\frac{1+x}{1-x}.$$

The algorithm used for the calculation of the inverse hyperbolic tangent is as follows:

$$s \leftarrow \circ(1+x)$$

$$t \leftarrow \circ(1-x)$$

$$u \leftarrow \circ(\frac{s}{t})$$

$$v \leftarrow \circ(\log u)$$

$$w \leftarrow \circ(\frac{1}{2}v)$$

Now, we have to bound the rounding error for each step of this algorithm. First, let consider the parity of hyperbolic arc tangent  $(\operatorname{atanh}(-x) = -\operatorname{atanh}(x))$ : the problem is reduced to calculate  $\operatorname{atanh} x$  with  $x \ge 0$ .

That shows the rounding error on the calculation of at anh x can be bound by  $(1+7\times 2^{2-\exp(v)}+2^{\exp(v)-\exp(t)-\exp(v)+3})$  ulp on the result. So, to calculate the size of intermediary variables, we have to add, at least,  $\lceil \log_2(1+7\times 2^{2-\exp(v)}+2^{\exp(x)-\exp(t)-\exp(v)+3}) \rceil$  bits the wanted precision.

#### 4.12. The arc-sine function.

- (1) We use the formula  $\arcsin x = \arctan \frac{x}{\sqrt{1-x^2}}$
- (2) When x is near 1 we will experience uncertainty problems:
- (3) If  $x = a(1 + \delta)$  with  $\delta$  being the relative error then we will have

$$1 - x = 1 - a - a\delta = (1 - a)\left[1 - \frac{a}{1 - a}\delta\right]$$

So when using the arc tangent programs we need to take into account that decrease in precision.

### 4.13. The arc-cosine function.

(1) Obviously, we used the formula

$$\arccos x = \frac{\pi}{2} - \arcsin x$$

- (2) The problem of arccos is that it is 0 at 1, so, we have a cancellation problem to treat at 1.
- (3) (Suppose  $x \ge 0$ , this is where the problem happens) The derivative of arccos is  $\frac{-1}{\sqrt{1-x^2}}$  and we will have

$$\frac{1}{2\sqrt{1-x}} \le \left| \frac{-1}{\sqrt{1-x^2}} \right| = \frac{1}{\sqrt{(1-x)(1+x)}} \le \frac{1}{\sqrt{1-x}}$$

So, integrating the above inequality on [x, 1] we get

$$\sqrt{1-x} \le \arccos x \le 2\sqrt{1-x}$$

(4) The important part is the lower bound that we get which tell us a upper bound on the cancellation that will occur:

The terms that are canceled are  $\pi/2$  and arcsin x, their order is 2. The number of canceled terms is so

$$1-1/2*MPFR_EXP(1-x)$$

4.14. **The arc-tangent function.** The arc-tangent function admits the following argument reduction:

$$\arctan x = 2\arctan \frac{x}{1 + \sqrt{1 + x^2}}.$$

If applied once, it reduced the argument to |x| < 1, then each successive application reduces x by a factor of at least 2.

4.14.1. Binary splitting. The Taylor series for arctan is suitable for analysis using Binary splitting.

This method is detailed for example in "Pi and The AGM" p 334. It is efficient for rational numbers and is non efficient for non rational numbers.

The efficiency of this method is then quite limited. One can then wonder how to use it for non rational numbers.

Using the formulas

$$\arctan(-x) = -\arctan x$$
 and  $\arctan x + \arctan \frac{1}{x} = \frac{\pi}{2} \operatorname{sign}(x)$ 

we can restrict ourselves to  $0 \le x \le 1$ .

Writing

$$x = \sum_{i=1}^{\infty} \frac{u_i}{2^i} \text{ with } u_i \in \{0, 1\}$$

or

$$x = \sum_{i=1}^{\infty} \frac{u_i}{2^{2^i}}$$
 with  $u_i \in \{0, 1, \dots, 2^{2^{i-1}}\}$  if  $i > 1$  and  $u_1 \in \{0, 1\}$ 

we can compute cos, sin or exp using the formulas

$$\cos(a+b) = \cos a \cos b - \sin a \sin b$$
  

$$\sin(a+b) = \sin a \cos b + \cos a \sin b$$
  

$$\exp(a+b) = (\exp a)(\exp b)$$

Unfortunately for arctan there is no similar formulas. The only formula known is

$$\arctan x + \arctan y = \arctan \frac{x+y}{1-xy} + k\pi \text{ with } k \in \mathcal{Z}$$

we will use

$$\arctan x = \arctan y + \arctan \frac{x-y}{1+xy}$$

with x, y > 0 and y < x.

Summarizing we have the following facts:

- (1) We can compute efficiently  $\arctan \frac{u}{2^{2^k}}$  with  $k \ge 0$  and  $u \in \{0, 1, \dots, 2^{2^{k-1}}\}$
- (2) We have a sort of addition formula for arctan, the term  $k\pi$  being zero.
- So I propose the following algorithm for x given in [0,1].
  - (1) Write  $v_k = 2^{2^k}$
  - (2) Define

$$s_{k+1} = \frac{s_k - A_k}{1 + s_k A_k}$$
 and  $s_0 = x$ 

(3)  $A_k$  is chosen such that

$$0 \le s_k - A_k < \frac{1}{v_k}$$

and  $A_k$  is of the form  $\frac{u_k}{v_k}$  with  $u_k \in \mathcal{N}$ .

(4) We have the formula

$$\arctan x = \arctan A_0 + \arctan s_1$$
  
=  $\arctan A_0 + \arctan A_1 + \arctan s_2$   
=  $\arctan A_0 + \dots + \arctan A_N + \arctan s_{N+1}$ 

the number  $s_N$  is decreasing toward 0 and we then have

$$\arctan x = \sum_{i=0}^{i=\infty} \arctan A_i$$

The drawbacks of this algorithm are:

- (1) Complexity of the process is high, higher than the AGM. Nevertheless there is some hope that this can be more efficient than AGM in the domain where the number of bits is high but not too large.
- (2) There is the need for division which is computationally expensive.
- (3) We may have to compute  $\arctan(1/2)$ .
- 4.14.2. Estimate of absolute error. By that analysis we mean that a and b have absolute error D if  $|a b| \le D$ .

I give a remind of the algorithm:

- (1) Write  $v_k = 2^{2^k}$
- (2) Define

$$s_{k+1} = \frac{s_k - A_k}{1 + s_k A_k}$$
 and  $s_0 = x$ 

(3)  $A_k$  is chosen such that

$$0 \le s_k - A_k < \frac{1}{v_k}$$

and  $A_k$  is of the form  $\frac{u_k}{v_k}$  with  $u_k \in \mathcal{N}$ .

(4) We have the formula

$$\arctan x = \arctan A_0 + \arctan s_1$$
  
=  $\arctan A_0 + \arctan A_1 + \arctan s_2$   
=  $\arctan A_0 + \cdots + \arctan A_N + \arctan s_{N+1}$ 

the number  $s_N$  is very rapidly decreasing toward 0 and we then have

$$\arctan x = \sum_{i=0}^{i=\infty} \arctan A_i$$

(5) The approximate arc tangent is then

$$\sum_{i=0}^{i=N_0} \arctan_{m_i} A_i$$

with  $\arctan_{m_i}$  being the sum of the first  $2^{m_i}$  terms of the Taylor series for arctan. We need to estimate all the quantities involved in the computation.

(1) We have the upper bound

$$0 \le s_{k+1} = \frac{s_k - A_k}{1 + s_k A_k} \le s_k - A_k \le \frac{1}{v_k}$$

(2) The remainder of the series giving  $\arctan x$  is

$$\sum_{i=N_0+1}^{\infty} \arctan A_i \leq \sum_{i=N_0+1}^{\infty} A_i$$

$$\leq \sum_{i=N_0+1}^{\infty} s_i$$

$$\leq \sum_{i=N_0+1}^{\infty} \frac{1}{v_{i-1}}$$

$$\leq \sum_{i=N_0}^{\infty} \frac{1}{v_i}$$

$$\leq \sum_{i=N_0}^{\infty} \frac{1}{2^{2^i}} = \frac{c_{N_0}}{2^{2^{N_0}}}$$

With  $c_{N_0} \leq 1.64$ . If  $N_0 \geq 1$  then  $c_{N_0} \leq 1.27$ . If  $N_0 \geq 2$  then  $c_{N_0} \leq 1.07$ . It remains to determine the right  $N_0$ .

- (3) The partial sum of the Taylor series for arctan have derivative bounded by 1 and consequently don't increase error.
- (4) The error created by using the partial sum of the Taylor series of arctan is bounded by

$$\frac{(A_i)^{2 \times 2^{m_i} + 1}}{2 * 2^{m_i} + 1}$$

and is thus bounded by

$$\frac{1}{2 \times 2^{m_i} + 1} \left[ \frac{1}{2^{2^{i-1}}} \right]^{2 \times 2^{m_i} + 1} = \frac{1}{2 \times 2^{m_i} + 1} \left[ 2^{-2^{i-1}} \right]^{2 \times 2^{m_i} + 1} \\
\leq \frac{1}{2 \times 2^{m_i} + 1} \left[ 2^{-2^{i-1}} \right]^{2 \times 2^{m_i}} \\
\leq \frac{1}{2 \times 2^{m_i} + 1} 2^{-2^{i+m_i}}$$

The calculation of  $\frac{\arctan A_i}{A_i}$  is done by using integer arithmetic and returning a fraction that is converted to mpfr type so there is no error. But to compute  $\arctan A_i = A_i[\frac{\arctan A_i}{A_i}]$  we need to use real arithmetic so there is 1ulp error. In total this is  $(N_0)ulp$ .

- (5) Addition give 1ulp There are  $(N_0 1)$  addition so we need to take  $(N_0 1)ulp$ .
- (6) The division yields errors:
  - (a) Having errors in the computation of  $A_i$  is of no consequences: It changes the quantity being arc-tangented and that's all. Errors concerning the computation of  $s_{N+1}$  in contrary adds to the error.
  - (b) The subtract operation  $s_i A_i$  has the effect of subtracting very near numbers. But  $A_i$  has exactly the same first 1 and 0 than  $s_i$  so we can expect this operation to be nondestructive.
  - (c) Extrapolating from the previous result we can expect that the error of the quantity  $\frac{s_i A_i}{1 + s_i A_i}$  is  $err(s_i) + 1ulp$
- (7) The total sum of errors is then (if no errors are done in the counting of errors)

$$Err(\arctan) = \sum_{i=0}^{i=N_0} \frac{1}{2 * 2^{m_i} + 1} 2^{-2^{i+m_i}} + \frac{c_{N_0}}{2^{2^{N_0}}} + (N_0 - 1) 2^{-Prec}$$

$$+ (N_0 - 1) 2^{-Prec} + (N_0) 2^{-Prec} \quad [m_i = N_0 - i]$$

$$= \sum_{i=0}^{i=N_0} \frac{1}{2 * 2^{N_0 - i} + 1} 2^{-2^{N_0}} + \frac{c_{N_0}}{2^{2^{N_0}}} + (3 * N_0 - 2) 2^{-Prec}$$

$$= \sum_{i=0}^{i=N_0} \frac{1}{2 * 2^i + 1} 2^{-2^{N_0}} + \frac{c_{N_0}}{2^{2^{N_0}}} + (3 * N_0 - 2) 2^{-Prec}$$

$$\leq \{\sum_{i=0}^{i=\infty} \frac{1}{2 * 2^i + 1}\} 2^{-2^{N_0}} + \frac{c_{N_0}}{2^{2^{N_0}}} + (3 * N_0 - 2) 2^{-Prec}$$

$$\leq \{0.77\} 2^{-2^{N_0}} + \frac{1.63}{2^{2^{N_0}}} + (3 * N_0 - 2) 2^{-Prec}$$

$$= \frac{2.4}{2^{2^{N_0}}} + (3 * N_0 - 2) 2^{-Prec}$$

This is what we wish thus  $Err(\arctan) < 2^{-prec\_arctan}$  with  $prec\_arctan$  is the requested precision on the arc-tangent. We thus want:

$$\frac{2.4}{2^{2^{N_0}}} \le 2^{-prec\_arctan - 1}$$

and

$$(3 \times N_0 - 2)2^{-Prec} \le 2^{-prec\_arctan - 1}$$

i.e.

$$N_0 \geq \frac{\ln \left(prec\_arctan + 1 + \frac{\ln 2.4}{\ln 2}\right)}{\ln 2}$$

that we approach by (since the logarithm is expensive):

$$N_0 = ceil(\log(prec\_arctan + 2.47) * 1.45)$$

and we finally have:

$$Prec = prec\_arctan + \{1 + ceil(\frac{\ln(3N_0 - 2)}{\ln 2})\}$$

4.14.3. Estimate of the relative error. we say that a and b have relative error  $\delta$  if

$$a = b(1 + \Delta)$$
 with  $|\Delta| \le \delta$ 

This is the error definition used in mpfr. So we need to redo everything in order to have a consistent analysis.

- (1) We can use all previous estimates:
  - (a) Remainder estimate:

$$\sum_{i=N_0+1}^{\infty} \arctan A_i \le \frac{c_{N_0}}{2^{2^{N_0}}}$$

so the relative error will be  $\frac{1}{\arctan x} \frac{c_{N_0}}{2^{2^{N_0}}}$ .

- (b) The relative error created by using a partial sum of Taylor series is bounded by  $\frac{1}{\arctan A_i} \frac{1}{2 \times 2^{m_i} + 1} 2^{-2^{i+m_i}}.$
- (c) The multiplication  $A_i = A_i \left[ \frac{\arctan A_i}{A_i} \right]$  takes 1 ulp of relative error.
- (d) Doing the subtraction  $s_i A_i$  is a gradual underflow operation: it decreases the precision of  $s_i A_i$ .
- (e) The multiplication  $a_iA_i$  creates 1 ulp of error. This is not much and this relative error is further reduced by adding 1.
- (1) We have

$$\begin{array}{rcl} \arctan\,b(1+\Delta) &=& \arctan(b+b\Delta) \\ &\sim& \arctan\,b+\frac{1}{1+b^2}(b\Delta) \\ &=& [\arctan\,b][1+\{\frac{b}{(1+b^2)\arctan\,b}\}\Delta] \end{array}$$

A rapid analysis gives  $0 \le \frac{b}{(1+b^2)\arctan b} \le 1$  and then we can say that the function arctan does not increase the relative error.

- (2) So we have two possible solutions:
  - (a) Do a relative analysis of our algorithm.
  - (b) Use the previous analysis since the absolute error D is obviously equal to  $|b|\delta$  ( $\delta$  being the relative error)

it is not hard to see that second solution is certainly better: The formulas are additive. Our analysis will work without problems.

(3) It then suffices to replace in the previous section  $2^{-prec\_arctan}$  by  $2^{-prec\_arctan}$  arctan x.

(4) If  $|x| \le 1$  then | arctan x| is bounded below by  $|x| \frac{4}{\pi} \sim |x| 1.27$ . So it suffices to have an absolute error bounded above by

$$2^{-prec\_arctan} |x| 1.27$$

In this case we will add  $2 - MPFR\_EXP(x)$  to  $prec\_arctan$ 

(5) If  $|x| \ge 1$  then  $\arctan x$  is bounded below by  $\frac{\pi}{4}$ . So it suffices to have an absolute error bounded above by

$$2^{-prec\_arctan}$$
 1.27

we will add 1 to prec\_arctan.

In this case we need to take into account the error caused by the subtraction:

$$\arctan x = \pm \frac{\pi}{2} - \arctan \frac{1}{x}$$

- 4.14.4. Implementation defaults.
  - (1) The computation is quite slow, this should be improved.
  - (2) The precision should be decreased after the operation  $s_i A_i$ . And several other improvement should be done.

4.15. **The Euclidean distance function.** The mpfr\_hypot function implements the Euclidean distance function:

$$hypot(x,y) = \sqrt{x^2 + y^2}.$$

If one of the variables is zero, then hypot is computed using the absolute value of the other variable. Assume that  $0 < y \le x$ . Using the first degree Taylor polynomial, we have:

$$0 < \sqrt{x^2 + y^2} - x < \frac{y^2}{2x}$$
.

Let  $p_x$ ,  $p_y$  be the precisions of the input variables x and y respectively,  $p_z$  the output precision and  $z = \circ_{p_z}(\sqrt{x^2 + y^2})$  the expected result. Let us assume, as it is the case in MPFR, that the minimal and maximal acceptable exponents (respectively  $e_{min}$  and  $e_{max}$ ) satisfy  $2 < e_{max}$  and  $e_{max} = -e_{min}$ .

When rounding to nearest, if  $p_x \leq p_z$  and  $\frac{p_z+1}{2} < \exp(x) - \exp(y)$ , we have  $\frac{y^2}{2x} < \frac{1}{2} \text{ulp}_{p_z}(x)$ ; if  $p_z < p_x$ , the condition  $\frac{p_x+1}{2} < \exp(x) - \exp(y)$  ensures that  $\frac{y^2}{2x} < \frac{1}{2} \text{ulp}_{p_x}(x)$ . In both cases, these inequalities show that  $z = \mathcal{N}_{p_z}(x)$ , except that tie case is rounded toward plus infinity since hypot(x,y) is strictly greater than x.

With the other rounding modes, the conditions  $p_z/2 < \exp(x) - \exp(y)$  if  $p_x \le p_z$ , and  $p_x/2 < \exp(x) - \exp(y)$  if  $p_z < p_x$  mean in a similar way that  $z = \circ_{p_z}(x)$ , except that we need to add one ulp to the result when rounding toward plus infinity and x is exactly representable with  $p_z$  bits of precision.

When none of the above conditions are satisfied and when  $\exp(x) - \exp(y) \le e_{max} - 2$ , we use the following algorithm:

Algorithm hypot\_1

Input: x and y with  $|y| \le |x|$ , p the working precision with  $p \ge p_z$ .

Output: 
$$\sqrt{x^2 + y^2}$$
 with  $\begin{cases} p - 4 \text{ bits of precision if } p < \max(p_x, p_y), \\ p - 2 \text{ bits of precision if } \max(p_x, p_y) \le p. \end{cases}$   
 $s \leftarrow \lfloor e_{max}/2 \rfloor - \operatorname{Exp}(x) - 1$   
 $x_s \leftarrow \mathcal{Z}(x \times 2^s)$ 

$$y_s \leftarrow \mathcal{Z}(y \times 2^s)$$

$$u \leftarrow \mathcal{Z}(x_s^2)$$

$$v \leftarrow \mathcal{Z}(y_s^2)$$

$$w \leftarrow \mathcal{Z}(u+v)$$

$$t \leftarrow \mathcal{Z}(\sqrt{w})$$

$$z \leftarrow \mathcal{Z}(t/2^s)$$

In order to avoid undue overflow during computation, we shift inputs' exponents by  $s = \lfloor \frac{e_{max}}{2} \rfloor - 1 - \operatorname{Exp}(x)$  before computing squares and shift back the output's exponent by -s using the fact that  $\sqrt{(x.2^s)^2 + (y.2^s)^2}/2^s = \sqrt{x^2 + y^2}$ . We show below that neither overflow nor underflow goes on.

We check first that the exponent shift does not cause overflow and, in the same time, that the squares of the shifted inputs never overflow. For x, we have  $\exp(x) + s = \lfloor e_{max}/2 \rfloor - 1$ , so  $\exp(x_s^2) < e_{max} - 1$  and neither  $x_s$  nor  $x_s^2$  overflows. For y, note that we have  $y_s \leq x_s$  because  $y \leq x$ , thus  $y_s$  and  $y_s^2$  do not overflow.

Secondly, let us see that the exponent shift does not cause underflow. For x, we know that  $0 \le \exp(x) + s$ , thus neither  $x_s$  nor  $x_s^2$  underflows. For y, the condition  $\exp(x) - \exp(y) \le e_{max} - 2$  ensures that  $-e_{max}/2 \le \exp(y) + s$  which shows that  $y_s$  and its square do not underflow.

Thirdly, the addition does not overflow because  $u + v < 2x_s^2$  and it was shown above that  $x_s^2 < 2^{e_{max}-1}$ . It cannot underflow because both operands are positive.

Fourthly, as  $x_s < t$ , the square root does not underflow. Due to the exponent shift, we have  $1 \le x_s$ , then w is greater than 1 and thus greater than its square root t, so the square root does overflow.

Finally, let us show that the back shift raises neither underflow nor overflow unless the exact result is greater than or equal to  $2^{e_{max}}$ . Because no underflow has occurred so far  $\exp(x) \leq \exp(t) - s$  which shows that it does not underflow. And all roundings being toward zero, we have  $z \leq \sqrt{x^2 + y^2}$ , so if  $2^{e_{max}} \leq z$ , then the exact value is also greater than or equal to  $2^{e_{max}}$ .

Let us analyse now the error of the algorithm hypot\_1:

```
p < \min(p_x, p_y) \mid \max(p_x, p_y) \le p
                                                                        \operatorname{error}(x_s) \leq \operatorname{error}(y_s) \leq \operatorname{error}(u) \leq \operatorname{error}(v) \leq \operatorname{error}(w) \leq \operatorname{error}(t) \leq \operatorname{error}(t)
x_s \leftarrow \mathcal{Z}(x \times 2^s)
                                                                                                                                       1 \operatorname{ulp}(x_s)
                                                                                                                                                                                                       exact
y_s \leftarrow \mathcal{Z}(y \times 2^s)
                                                                                                                                       1 \text{ ulp}(y_s)
                                                                                                                                                                                                       exact
u \leftarrow \mathcal{Z}(x_s^2)
                                                                                                                                         6 \operatorname{ulp}(u)
                                                                                                                                                                                               1 \operatorname{ulp}(u)
v \leftarrow \mathcal{Z}(y_s^2)
                                                                                                                                          6 \operatorname{ulp}(v)
                                                                                                                                                                                               1 \operatorname{ulp}(v)
w \leftarrow \mathcal{Z}(u+v)
                                                                                                                                     13 \operatorname{ulp}(w)
                                                                                                                                                                                             3 \operatorname{ulp}(w)
t \leftarrow \mathcal{Z}(\sqrt{w})
                                                                                                                                        14 \operatorname{ulp}(t)
                                                                                                                                                                                                4 \operatorname{ulp}(t)
z \leftarrow \mathcal{Z}(t/2^s)
                                                                         exact.
```

And in the intermediate case, if  $\min(p_x, p_y) \leq p < \max(p_x, p_y)$ , we have

Thus, 2 bits of precision are lost when  $\max(p_x, p_y) \leq p$  and 4 bits when p does not satisfy this relation.

4.16. The floating multiply-add function. The mpfr\_fma (fma(x, y, z)) function implements the floating multiply-add function as:

$$fma(x, y, z) = z + x \times y.$$

The algorithm used for this calculation is as follows:

$$\begin{array}{rcl} u & \leftarrow & \circ(x \times y) \\ v & \leftarrow & \circ(z+u) \end{array}$$

Now, we have to bound the rounding error for each step of this algorithm.

$$\begin{aligned} & \operatorname{error}(u) \\ & u \leftarrow \circ(x \times y) \end{aligned} \qquad |u - (xy)| & \leq u l p(u) \\ & \operatorname{error}(v) \\ & v \leftarrow \circ(z + u) \end{aligned} \qquad |v - (z + xy)| & \leq u l p(v) + |(z + u) - (z + xy)| \\ & \leq (1 + 2^{e_u - e_v}) u l p(v) \quad (\star) \end{aligned} \qquad \text{see subsection 2.3}$$

That shows the rounding error on the calculation of  $\operatorname{fma}(x, y, z)$  can be bound by  $(1 + 2^{e_u - e_v})$ ulp on the result. So, to calculate the size of intermediary variables, we have to add, at least,  $\lceil \log_2(1 + 2^{e_u - e_v}) \rceil$  bits the wanted precision.

4.17. **The expm1 function.** The  $mpfr_expm1$  (expm1(x)) function implements the expm1 function as:

$$\operatorname{expm1}(x) = e^x - 1.$$

The algorithm used for this calculation is as follows:

$$u \leftarrow \circ(e^x)$$

$$v \leftarrow \circ(u-1)$$

Now, we have to bound the rounding error for each step of this algorithm.

$$\begin{array}{ll} \operatorname{error}(u) & |u - e^x| \leq u l p(u) \\ u \leftarrow \circ(e^x) & \\ \operatorname{error}(v) & (\star) \\ v \leftarrow \circ(u-1) & |v - (e^x - 1)| \leq (1 + 2^{e_u - e_v}) \operatorname{ulp}(v) & (\star) & \text{see subsection 2.3} \end{array}$$

That shows the rounding error on the calculation of expm1(x) can be bound by  $(1 + 2^{e_u - e_v})$ ulp on the result. So, to calculate the size of intermediary variables, we have to add, at least,  $\lceil \log_2(1 + 2^{e_u - e_v}) \rceil$  bits the wanted precision.

4.18. The log1p function. The mpfr\_log1p function implements the log1p function as:

$$\log 1p(x) = \log(1+x).$$

We could use the argument reduction

$$\log 1p(x) = 2\log 1p\left(\frac{x}{1+\sqrt{1+x}}\right),\,$$

which reduces x to about  $\sqrt{x}$  when  $x \gg 1$ , and in any case to less than x/2 when x > 0. However, if 1+x can be computed exactly with the target precision, then it is more efficient to directly call the logarithm, which has its own argument reduction. If 1+x cannot be computed exactly, this implies that x is either very small, in which case no argument reduction is needed, or very large, in which case  $\log 1p(x) \approx \log x$ .

The algorithm used for this calculation is as follows (with rounding to nearest):

$$v \leftarrow \circ (1+x)$$
$$w \leftarrow \circ (\log v)$$

Now, we have to bound the rounding error for each step of this algorithm.

$$\begin{array}{lll} \operatorname{error}(v) & & & |v - (1+x)| & \leq & \frac{1}{2} \operatorname{ulp}(v) \\ \operatorname{error}(w) & & & |w - \log(1+x)| & \leq & (\frac{1}{2} + 2^{1-e_w}) \operatorname{ulp}(w) & (\star) \text{ see subsection } 2.9 \end{array}$$

The  $2^{1-e_w}$  factor in the error reflects the possible loss of accuracy in 1+x when x is small. Note that if v = o(1+x) is exact, then the error bound simplifies to  $2^{1-e_w} \text{ulp}(w)$ , i.e.,  $2^{1-p}$ , where p is the working precision.

4.19. **The log2 or log10 function.** The mpfr\_log2 or mpfr\_log10 function implements the log in base 2 or 10 function as:

$$\log 2(x) = \frac{\log x}{\log 2}$$

or

$$\log 10(x) = \frac{\log x}{\log 10}.$$

The algorithm used for this calculation is the same for  $\log 2$  or  $\log 10$  and is described as follows for t = 2 or 10:

$$\begin{array}{rcl} u & \leftarrow & \circ(\log(x)) \\ v & \leftarrow & \circ(\log(t)) \\ w & \leftarrow & \circ(\frac{u}{v}) \end{array}$$

Now, we have to bound the rounding error for each step of this algorithm with  $x \ge 0$  and y is a floating number.

$$\begin{array}{lll} \operatorname{error}(u) & & & & \\ u & \leftarrow & & \\ \triangle(\log(x)) & & |u - \log(x)| & \leq & \operatorname{ulp}(u) \\ (\bullet) & & & \\ \operatorname{error}(v) & & & \\ v \leftarrow \nabla(\log t) & & |v - \log t| & \leq & \operatorname{ulp}(v) \\ (\bullet \bullet) & & & |v - (\frac{\log x}{\log t})| & \leq & \operatorname{5ulp}(w) \ \ (\star) & & \operatorname{see subsection } 2.6 \end{array}$$

That shows the rounding error on the calculation of log2 or log10 can be bound by 5ulp on the result. So, to calculate the size of intermediary variables, we have to add, at least, 3 bits the wanted precision.

#### 4.20. The power function. The mpfr\_pow function implements the power function as:

$$pow(x, y) = e^{y \log(x)}.$$

The algorithm used for this calculation is as follows:

$$u \leftarrow \circ(\log(x))$$

$$v \leftarrow \circ(yu)$$

$$w \leftarrow \circ(e^v)$$

Now, we have to bound the rounding error for each step of this algorithm with  $x \ge 0$  and y is a floating number.

$$\begin{array}{lll} \operatorname{error}(u) & u & \leftarrow & |u - \log(x)| & \leq & \operatorname{ulp}(u) & \star \\ & \circ (\log(x)) & |v - y \log(x)| & \leq & \operatorname{ulp}(v) + |yu - y \log(x)| & (\star) \\ & \operatorname{error}(v) & & \leq & \operatorname{ulp}(v) + y|u - \log(x)| & \operatorname{with} & [\operatorname{Rule} \ 4] \\ & v \leftarrow \triangle(y \times u) & \leq & \operatorname{ulp}(v) + y \operatorname{ulp}(u) & (\star) \\ & \leq & \operatorname{ulp}(v) + 2 \operatorname{ulp}(yu) & (\star) & \operatorname{with} & [\operatorname{Rule} \ 8] \\ & \leq & \operatorname{3ulp}(v) & (\star\star) & \\ & \operatorname{error}(w) & & (\star) \text{ see subsection 2.8} \\ & w \leftarrow \circ(e^v) & |w - e^v| & \leq & (1 + 3 \cdot 2^{\operatorname{exp}(v) + 1}) \operatorname{ulp}(w) & \operatorname{with} \ c_u^* = 1 \text{ for } (\bullet) \end{array}$$

That shows the rounding error on the calculation of  $x^y$  can be bound by  $1 + 3 \cdot 2^{\exp(v)+1}$  ulps on the result. So, to calculate the size of intermediary variables, we have to add, at least,  $\lceil \log_2(1+3\cdot 2^{\exp(v)+1}) \rceil$  bits to the wanted precision.

EXACT RESULTS. We have to detect cases where  $x^y$  is exact, otherwise the program will loop forever. The theorem from Gelfond/Schneider (1934) states that if  $\alpha$  and  $\beta$  are algebraic numbers with  $\alpha \neq 0$ ,  $\alpha \neq 1$ , and  $\beta \notin \mathbb{Q}$ , then  $\alpha^{\beta}$  is transcendental. This is of little help for us

since  $\beta$  will always be a rational number. Let  $x = a2^b$ ,  $y = c2^d$ , and assume  $x^y = e2^f$ , where a, b, c, d, e, f are integers. Without loss of generality, we can assume a, c, e odd integers.

If x is negative: either y is integer, then  $x^y$  is exact if and only if  $(-x)^y$  is exact; or y is rational, then  $x^y$  is a complex number, and the answer is NaN (Not a Number). Thus we can assume a (and therefore e) positive.

If y is negative, then  $x^y = a^y 2^{by}$  can be exact only when a = 1, and in that case we also need that by is an integer.

We have  $a^{c2^d}2^{bc2^d} = e2^f$  with a, c, e odd integers, and a, e > 0. As a is an odd integer, necessarily we have  $a^{c2^d} = e$  and  $2^{bc2^d} = 2^f$ , thus  $bc2^d = f$ .

If  $d \ge 0$ , then  $a^c$  must be an integer: this is true if  $c \ge 0$ , and false for c < 0 since  $a^{c2^d} = \frac{1}{a^{-c2^d}} < 1$  cannot be an integer. In addition  $a^{c2^d}$  must be representable in the given precision.

Assume now d < 0, then  $a^{c2^d} = a^{c1/2^{d'}}$  with d' = -d, thus we have  $a^c = e^{2^{d'}}$ , thus  $a^c$  must be a  $2^{d'}$ -th power of an integer. Since c is odd, a itself must be a  $2^{d'}$ -th power.

We therefore propose the following algorithm:

```
Algorithm CheckExactPower.

Input: x = a2^b, y = c2^d, a, c odd integers

Output: true if x^y is an exact power e2^f, false otherwise

if x < 0 then

if y is an integer then return CheckExactPower(-x, y)

else return false

if y < 0 then

if y < 0 then
```

Detecting if the result is exactly representable is not enough, since it may be exact, but with a precision larger than the target precision. Thus we propose the following: modify Algorithm CheckExactPower so that it returns an upper bound p for the number of significant bits of  $x^y$  when it is exactly representable, i.e.  $x^y = m \cdot 2^e$  with  $|m| < 2^p$ . Then if the relative error on the approximation of  $x^y$  is less than  $\frac{1}{2}$  ulp, then rounding it to nearest will give  $x^y$ .

4.21. The real cube root. The mpfr\_cbrt function computes the real cube root of x. Since for x < 0, we have  $\sqrt[3]{x} = -\sqrt[3]{-x}$ , we can focus on x > 0.

Let n be the number of wanted bits of the result. We write  $x=m\cdot 2^{3e}$  where m is a positive integer with  $m\geq 2^{3n-3}$ . Then we compute the integer cubic root of m: let  $m=s^3+r$  with  $0\leq r$  and  $m<(s+1)^3$ . Let k be the number of bits of s: since  $m\geq 2^{3n-3}$ , we have  $s\geq 2^{n-1}$  thus  $k\geq n$ . If k>n, we replace s by  $\lfloor s2^{n-k}\rfloor$ , e by e+(k-n), and update r accordingly so that  $x=(s^3+r)2^{3e}$  still holds (be careful that r may no longer be an integer in that case).

Then the correct rounding of  $\sqrt[3]{x}$  is:

```
s2^e if r=0 or round down or round nearest and r<\frac{3}{2}s^2+\frac{3}{4}s+\frac{1}{8}, (s+1)2^e otherwise.
```

Note: for rounding to nearest, one may consider  $m \ge 2^{3n}$  instead of  $m \ge 2^{3n-3}$ , i.e. taking n+1 instead of n. In that case, there is no need to compare the remainder  $n \ge 2^{3n-3}$ , i.e. taking n+1 instead of n. In that case, there is no need to compare the remainder  $n \ge 2^{3n-3}$ , i.e. taking

we just need to know whether r = 0 or not. The even rounding rule is needed only when the input x has at least 3n + 1 bits, since the cube of a odd number of n + 1 bits has at least 3n + 1 bits.

4.22. The exponential integral. The exponential integral mpfr\_eint is defined as in [1, formula 5.1.10]: for x > 0,

$$\mathrm{Ei}(x) = \gamma + \log x + \sum_{k=1}^{\infty} \frac{x^k}{k \, k!},$$

and for x < 0 it gives NaN.

We use the following integer-based algorithm to evaluate  $\sum_{k=1}^{\infty} \frac{x^k}{k \, k!}$ , using working precision w. For any real v, we denote by  $\operatorname{trunc}(v)$  the nearest integer toward zero.

Decompose x into  $m \cdot 2^e$  with m integer [exact] If necessary, truncate m to w bits and adjust e  $s \leftarrow 0$   $t \leftarrow 2^w$  for k := 1 do  $t \leftarrow \operatorname{trunc}(tm2^e/k)$   $u \leftarrow \operatorname{trunc}(t/k)$   $s \leftarrow s + u$  Return  $s \cdot 2^{-w}$ .

Note: in  $t \leftarrow \operatorname{trunc}(tm2^e/k)$ , we first compute tm exactly, then if e is negative, we first divide by  $2^{-e}$  and truncate, then divide by k and truncate; this gives the same answer than dividing once by  $k2^{-e}$ , but it is more efficient. Let  $\epsilon_k$  be the absolute difference between t and  $2^w x^k/k!$  at step k. We have  $\epsilon_0 = 0$ , and  $\epsilon_k \leq 1 + \epsilon_{k-1} m 2^e/k + t_{k-1} m 2^{e+1-w}/k$ , since the error when approximating x by  $m2^e$  is less than  $m2^{e+1-w}$ . Similarly, the absolute error on e at step e is at most e in e is at most e is at most e in e

At that time, the truncation error when neglecting terms of index k+1 to  $\infty$  can be bounded by  $(|t| + \epsilon_k)/k(|x|/k + |x|^2/k^2 + \cdots) \le (|t| + \epsilon_k)|x|/k/(k - |x|)$ . Asymptotic Expansion. For  $x \to \infty$  we have the following non-converging expansion [1, formula 5.1.51]:

$$\operatorname{Ei}(x) \sim e^x (\frac{1}{x} + \frac{1}{x^2} + \frac{2}{x^3} + \frac{6}{x^4} + \frac{24}{x^5} + \cdots).$$

The kth is of the form  $k!x^{-k-1}$ . The smallest value is obtained for  $k \approx x$ , and is of the order of  $e^{-x}$ . Thus assuming the error term is bounded by the first neglected term, we can use that expansion as long as  $e^{-x} \leq 2^{-p}$  where p is the target precision, i.e. when  $x \geq p \log 2$ .

4.23. The gamma function. The gamma function is computed by Spouge's method [22]:

$$\Gamma(z+1) \approx (z+a)^{z+1/2} e^{-z-a} \left[ \sqrt{2\pi} + \sum_{k=1}^{\lceil a \rceil - 1} \frac{c_k(a)}{z+k} \right],$$

which is valid for  $\Re(z+a)>0$ , where

$$c_k(a) = \frac{(-1)^{k-1}}{(k-1)!} (a-k)^{k-1/2} e^{a-k}.$$

Here, we choose the free parameter a to be an integer.

According to [18, Section 2.6], the relative error is bounded by  $a^{-1/2}(2\pi)^{-a-1/2}$  for  $a \ge 3$  and  $\Re(z) \ge 0$ . See also [21].

4.24. The Riemann Zeta function. The algorithm for the Riemann Zeta function is due to Jean-Luc Rémy and Sapphorain Pétermann [16, 17]. For s < 1/2 we use the functional equation

$$\zeta(s) = 2^{s} \pi^{s-1} \sin\left(\frac{\pi s}{2}\right) \Gamma(1-s) \zeta(1-s).$$

For  $s \ge 1/2$  we use the Euler-MacLaurin summation formula, applied to the real function  $f(x) = x^{-s}$  for s > 1:

$$\zeta(s) = \sum_{k=1}^{N-1} \frac{1}{k^s} + \frac{1}{2N^s} + \frac{1}{(s-1)N^{s-1}} + \sum_{k=1}^{p} \frac{B_{2k}}{2k} \binom{s+2k-2}{2k-1} \frac{1}{N^{s+2k-1}} + R_{N,p}(s),$$

with  $|R_{N,p}(s)| < 2^{-d}$ , where  $B_k$  denotes the kth Bernoulli number,

$$p = \max\left(0, \lceil \frac{d\log 2 + 0.61 + s\log(2\pi/s)}{2} \rceil\right),$$

and  $N = \lceil 2^{(d-1)/s} \rceil$  if p = 0,  $N = \lceil \frac{s+2p-1}{2\pi} \rceil$  if p > 0.

This computation is split into three parts:

$$A = \sum_{k=1}^{N-1} k^{-s} + \frac{1}{2} N^{-s},$$

$$B = \sum_{k=1}^{p} T_k = N^{-1-s} s \sum_{k=1}^{p} C_k \Pi_k N^{-2k+2},$$

$$C = \frac{N^{-s+1}}{s-1},$$

where  $C_k = \frac{B_{2k}}{(2k)!}$ ,  $\Pi_k = \prod_{j=1}^{2k-2} (s+j)$ , and  $T_k = N^{1-2k-s} C_k \Pi_k$ .

Rémy and Pétermann proved the following result:

**Theorem 1.** Let d be the target precision so that  $|R_{N,p}(s)| < 2^{-d}$ . Assume  $\Pi = d - 2 \ge 11$ , i.e.  $d \ge 13$ . If the internal precisions for computing A, B, C satisfy respectively

$$D_A \ge \Pi + \lceil \frac{3}{2} \frac{\log N}{\log 2} \rceil + 5, \quad D_B \ge \Pi + 14, \quad D_C \ge \Pi + \lceil \frac{1}{2} \frac{\log N}{\log 2} \rceil + 7,$$

then the relative round-off error is bounded by  $2^{-\Pi}$ , i.e. if z is the approximation computed, we have

$$|\zeta(s) - z| \le 2^{-\Pi} |\zeta(s)|.$$

4.24.1. The integer argument case. In case of an integer argument  $s \ge 2$ , the mpfr\_zeta\_ui function computes  $\zeta(s)$  using the following formula from [3]:

$$\zeta(s) = \frac{1}{d_n(1-2^{1-s})} \sum_{k=0}^{n-1} \frac{(-1)^k (d_n - d_k)}{(k+1)^s} + \gamma_n(s),$$

where

$$|\gamma_n(s)| \le \frac{3}{(3+\sqrt{8})^n} \frac{1}{1-2^{1-s}}$$
 and  $d_k = n \sum_{i=0}^k \frac{(n+i-1)!4^i}{(n-i)!(2i)!}$ .

It can be checked that the  $d_k$  are integers, and we compute them exactly, like the denominators  $(k+1)^s$ . We compute the integer

$$S = \sum_{k=0}^{n-1} (-1)^k \lfloor \frac{d_n - d_k}{(k+1)^s} \rfloor.$$

The absolute error on S is at most n. We then perform the following iteration (still with integers):

$$\begin{split} T &\leftarrow S \\ \mathbf{do} \\ T &\leftarrow \lfloor T2^{1-s} \rfloor \\ S &= S + T \\ \mathbf{while} \ T \neq 0. \end{split}$$

Since  $\frac{1}{1-2^{1-s}} = 1 + 2^{1-s} + 2^{2(1-s)} + \cdots$ , and at iteration i we have  $T = \lfloor S2^{i(1-s)} \rfloor$ , the error on S after this loop is bounded by n + l + 1, where l is the number of loops.

Finally we compute  $q = \lfloor \frac{2^p S}{d_n} \rfloor$ , where p is the working precision, and we convert q to a p-bit floating-point value, with rounding to nearest, and divide by  $2^p$  (this last operation is exact). The final error in ulps is bounded by  $1+2^\mu(n+l+2)$ . Since  $S/d_n$  approximates  $\zeta(s)$ , it is larger than one, thus  $q \geq 2^p$ , and the error on the division is less that  $\frac{1}{2}\mathrm{ulp}_p(q)$ . The error on S itself is bounded by  $(n+l+1)/d_n \leq (n+l+1)2^{1-p}$ — see the conjecture below. Since  $2^{1-p} \leq \mathrm{ulp}_p(q)$ , and taking into account the error when converting the integer q (which may have more than p bits), and the mathematical error which is bounded by  $\frac{3}{(3+\sqrt{8})^n} \leq \frac{3}{2^p}$ , the total error is bounded by n+l+4 ulps.

Analysis of the sizes. To get an accuracy of around p bits, since  $\zeta(s) \geq 1$ , it suffices to have  $|\gamma_n(s)| \leq 2^{-p}$ , i.e.  $(3+\sqrt{8})^n \geq 2^p$ , thus  $n \geq \alpha p$  with  $\alpha = \frac{\log 2}{\log((3+\sqrt{8})} \approx 0.393$ . It can be easily seen that  $d_n \geq 4^n$ , thus when  $n \geq \alpha p$ ,  $d_n$  has at least 0.786p bits. In fact, we conjecture  $d_n \geq 2^{p-1}$  when  $n \geq \alpha p$ ; this conjecture was experimentally verified up to p = 1000.

Large argument case. When  $3^{-s} < 2^{-p}$ , then  $\zeta(s) \approx 1 + 2^{-s}$  to a precision of p bits. More precisely, let  $r(s) := \zeta(s) - (1 + 2^{-s}) = 3^{-s} + 4^{-s} + \cdots$ . The function  $3^s r(s) = 1 + (3/4)^s + (3/5)^s + \cdots$  decreases with s, thus for  $s \ge 2$ ,  $3^s r(s) \le 3^2 \cdot r(2) < 4$ . This yields:

$$|\zeta(s) - (1+2^{-s})| < 4 \cdot 3^{-s}.$$

If the upper bound  $4 \cdot 3^{-s}$  is less than  $\frac{1}{2}\text{ulp}(1) = 2^{-p}$ , the correct rounding of  $\zeta(s)$  is either  $1 + 2^{-s}$  for rounding to zero,  $-\infty$  or nearest, and  $1 + 2^{-s} + 2^{1-p}$  for rounding to  $+\infty$ .

4.25. The arithmetic-geometric mean. The arithmetic-geometric mean (AGM for short) of two positive numbers  $a \leq b$  is defined to be the common limits of the sequences  $(a_n)$  and  $(b_n)$  defined by  $a_0 = a$ ,  $b_0 = b$ , and for  $n \geq 0$ :

$$a_{n+1} = \sqrt{a_n b_n}, \quad b_{n+1} = \frac{a_n + b_n}{2}.$$

We approximate AGM(a, b) as follows, with working precision p:

```
s_1 = \circ(ab)
u_1 = \circ(\sqrt{s_1})
v_1 = \circ(a+b)/2 \text{ [division by 2 is exact]}
for n := 1 while \exp(v_n) - \exp(v_n - u_n) \le p - 2 do
v_{n+1} = \circ(u_n + v_n)/2 \text{ [division by 2 is exact]}
if \exp(v_n) - \exp(v_n - u_n) \le p/4 then
s = \circ(u_n v_n)
u_{n+1} = \circ(\sqrt{s})
else
s = \circ(v_n - u_n)
t = \circ(s^2)/16 \text{ [division by 16 is exact]}
w = \circ(t/v_{n+1})
\text{return } r = \circ(v_{n+1} - w)
endif
```

The rationale behind the **if**-test is the following. When the relative error between  $a_n$  and  $b_n$  is less than  $2^{-p/4}$ , we can write  $a_n = b_n(1+\epsilon)$  with  $|\epsilon| \le 2^{-p/4}$ . The next iteration will compute  $a_{n+1} = \sqrt{a_n b_n} = b_n \sqrt{1+\epsilon}$ , and  $b_{n+1} = (a_n + b_n)/2 = b_n(1+\epsilon/2)$ . The second iteration will compute  $a_{n+2} = \sqrt{a_{n+1}b_{n+1}} = b_n \sqrt{\sqrt{1+\epsilon}(1+\epsilon/2)}$ , and  $b_{n+2} = (a_{n+1} + b_{n+1})/2 = b_n(\sqrt{1+\epsilon}/2+1/2+\epsilon/4)$ . When  $\epsilon$  goes to zero, the following expansions hold:

$$\sqrt{\sqrt{1+\epsilon}(1+\epsilon/2)} = 1 + \frac{1}{2}\epsilon - \frac{1}{16}\epsilon^2 + \frac{1}{32}\epsilon^3 - \frac{11}{512}\epsilon^4 + O(\epsilon^5) 
\sqrt{1+\epsilon}/2 + 1/2 + \epsilon/4 = 1 + \frac{1}{2}\epsilon - \frac{1}{16}\epsilon^2 + \frac{1}{32}\epsilon^3 - \frac{5}{256}\epsilon^4 + O(\epsilon^5),$$

which shows that  $a_{n+2}$  and  $b_{n+2}$  agree to p bits. In the algorithm above, we have  $v_{n+1} \approx b_n(1+\epsilon/2)$ ,  $s=-b_n\epsilon$  [exact thanks to Sterbenz theorem], then  $t\approx \epsilon^2 b_n^2/16$ , and  $w\approx (b_n/16)\epsilon^2/(1+\epsilon/2)\approx b_n(\epsilon^2/16-\epsilon^3/32)$ , thus  $v_{n+1}-w$  gives us an approximation to order  $\epsilon^4$ . [Note that w— and therefore s,t— need to be computed to precision p/2 only.]

**Lemma 6.** Assuming  $u \le v$  are two p-bit floating-point numbers, then  $u' = o(\sqrt{o(uv)})$  and v' = o(u+v)/2 satisfy:

$$u \le u', v' \le v.$$

*Proof.* It is clear that  $2u \le u + v \le 2v$ , and since 2u and 2v are representable numbers,  $2u \le o(u+v) \le 2v$ , thus  $u \le v' \le v$ .

The result for u' is more difficult to obtain. We use the following result: if x is a p-bit number,  $s = o(x^2)$ , and  $t = o(\sqrt{s})$  are computed with precision p and rounding to nearest, then t = x.

Apply this result to x = u, and let  $s' = \circ(uv)$ . Then  $s = \circ(u^2) \le s'$ , thus  $u = \circ(\sqrt{s}) \le \circ(\sqrt{s'}) = u'$ . We prove similarly that  $u' \le v$ .

Remark. We cannot assume that  $u' \le v'$ . Take for example u = 9, v = 12, with precision p = 4. Then (u + v)/2 rounds to 10, whereas  $\sqrt{uv}$  rounds to 112, and  $\sqrt{112}$  rounds to 11.

We use Higham error analysis method, where  $\theta$  denotes a generic value such that  $|\theta| \leq 2^{-p}$ . We note  $a_n$  and  $b_n$  the exact values we would obtain for  $u_n$  and  $v_n$  respectively, without round-off errors. We have  $s_1 = ab(1+\theta)$ ,  $u_1 = a_1(1+\theta)^{3/2}$ ,  $v_1 = b_1(1+\theta)$ . Assume we can write  $u_n = a_n(1+\theta)^{\alpha}$  and  $v_n = b_n(1+\theta)^{\beta}$  with  $\alpha, \beta \leq e_n$ . We thus can take  $e_1 = 3/2$ . Then as long as the **if**-condition is not satisfied,  $v_{n+1} = b_{n+1}(1+\theta)^{e_n+1}$ , and  $u_{n+1} = a_{n+1}(1+\theta)^{e_n+3/2}$ , which proves that  $e_n \leq 3n/2$ .

When the **if**-condition is satisfied, we have  $\exp(v_n - u_n) < \exp(v_n) - p/4$ , and since exponents are integers, thus  $\exp(v_n - u_n) \le \exp(v_n) - (p+1)/4$ , i.e.  $|v_n - u_n|/v_n < 2^{(3-p)/4}$ .

Assume  $n \leq 2^{p/4}$ , which implies  $3n|\theta|/2 \leq 1$ , which since  $n \geq 1$  implies in turn  $|\theta| \leq 2/3$ . Under that hypothesis,  $(1+\theta)^{3n/2}$  can be written  $1+3n\theta$  (possibly with a different  $|\theta| \leq 2^{-p}$  as usual). Then  $|b_n - a_n| = |v_n(1+3n\theta) - u_n(1+3n\theta')| \leq |v_n - u_n| + 3n|\theta|v_n$ .

For  $p \ge 4$ ,  $3n|\theta| \le 3/8$ , and 1/(1+x) for  $|x| \le 3/8$  can be written 1 + 5x'/3 for x' in the same interval. This yields:

$$\frac{|b_n - a_n|}{b_n} = \frac{|v_n - u_n| + 3n|\theta|v_n}{v_n(1+3n\theta)} \le \frac{|v_n - u_n|}{v_n} + 5n|\theta| \frac{|v_n - u_n|}{v_n} + \frac{8}{5}(6n\theta)$$

$$\le \frac{13}{8} \cdot 2^{(3-p)/4} + \frac{48}{5} \cdot 2^{-3p/4} \le 5 \cdot 2 \cdot 2^{-p/4}.$$

Write  $a_n = b_n (1 + \epsilon)$  with  $|\epsilon| \le 5.2 \cdot 2^{-p/4}$ . We have  $a_{n+1} = b_n \sqrt{1 + \epsilon}$  and  $b_{n+1} = b_n (1 + \epsilon/2)$ . Since  $\sqrt{1 + \epsilon} = 1 + \epsilon/2 - \frac{1}{8}\nu^2$  with  $|\nu| \le |\epsilon|$ , we deduce that  $|b_{n+1} - a_{n+1}| \le \frac{1}{8}\nu^2 |b_n| \le 3.38 \cdot 2^{-p/2} b_n$ . After one second iteration, we get similarly  $|b_{n+2} - a_{n+2}| \le \frac{1}{8} (3.38 \cdot 2^{-p/2})^2 b_n \le \frac{3}{2} 2^{-p} b_n$ .

Let q be the precision used to evaluate s, t and w in the **else** case. Since  $|v_n - u_n| \le 2^{(3-p)/4}v_n$ , it follows  $|s| \le 1.8 \cdot 2^{-p/4}v_n$  for  $q \ge 4$ . Then  $t \le 0.22 \cdot 2^{-p/2}v_n$ . Finally due to the above Lemma, the difference between  $v_{n+1}$  and  $v_n$  is less than that between  $u_n$  and  $v_n$ , i.e.  $\frac{v_n}{v_{n+1}} \le \frac{1}{1-2^{(3-p)/4}} \le 2$  for  $p \ge 7$ . We deduce  $w \le 0.22 \cdot 2^{-p/2} \frac{v_n^2}{v_{n+1}} (1+2^{-q}) \le 0.47 \cdot 2^{-p/2} v_n \le 0.94 \cdot 2^{-p/2} v_{n+1}$ .

The total error is bounded by the sum of four terms:

- the difference between  $a_{n+2}$  and  $b_{n+2}$ , bounded by  $\frac{3}{2}2^{-p}b_n$ ;
- the difference between  $b_{n+2}$  and  $v_{n+2}$ , if  $v_{n+2}$  was computed directly without the final optimization; since  $v_{n+2} = b_{n+2}(1+\theta)^{3(n+2)/2}$ , if  $n+2 \le 2^{p/4}$ , similarly as above,  $(1+\theta)^{3(n+2)/2}$  can be written  $1+3(n+2)\theta$ , thus this difference is bounded by  $3(n+2) \cdot 2^{-p}b_{n+2} \le 3(n+2) \cdot 2^{-p}b_n$ ;
- the difference between  $v_{n+2}$  computed directly, and with the final optimization. We can assume  $v_{n+2}$  is computed directly in infinite precision, since we already took into account the rounding errors above. Thus we want to compute the difference between

$$\frac{\sqrt{u_n v_n} + \frac{u_n + v_n}{2}}{2}$$
 and  $\frac{u_n + v_n}{2} - \frac{(v_n - u_n)^2}{8(u_n + v_n)}$ .

Writing  $u_n = v_n(1 + \epsilon)$ , this simplifies to:

$$\frac{\sqrt{1+\epsilon}+1+\epsilon/2}{2} - \left(\frac{1+\epsilon/2}{2} - \frac{\epsilon^2}{18+8\epsilon}\right) = \frac{-1}{256}\epsilon^4 + O(\epsilon^5).$$

For  $|\epsilon| \leq 1/2$ , the difference is bounded by  $\frac{1}{100} \epsilon^4 v_n \leq \frac{1}{100} 2^{3-p} v_n$ .

• the round-off error on w, assuming  $u_n$  and  $v_n$  are exact; we can write  $s = (v_n - u_n)(1+\theta)$ ,  $t = \frac{1}{16}(v_n - u_n)^2(1+\theta)^2$ ,  $w = \frac{(v_n - u_n)^2}{16v_{n+1}}(1+\theta)^4$ . For  $q \ge 4$ ,  $(1+\theta)^4$  can be written  $1+5\theta$ , thus the round-off error on w is bounded by  $5\theta w \le 4.7 \cdot 2^{-p/2-q} v_{n+1}$ . For  $q \ge p/2$ , this gives a bound of  $4.7 \cdot 2^{-p} v_{n+1}$ .

Since  $b_n = v_n(1+3n\theta)$ , and we assumed  $3n|\theta|/2 \le 1$ , we have  $b_n \le 3v_n$ , thus the first two errors are less than  $(9n+45/2)2^{-p}v_n$ ; together with the third one, this gives a bound of  $(9n+23)2^{-p}v_n$ ; finally since we proved above that  $v_n \le 2v_{n+1}$ , this gives a total bound of  $(18n+51)2^{-p}v_{n+1}$ , which is less than (18n+51)ulp(r), or twice this in the improbable case where there is an exponent loss in the final subtraction  $r = \circ(v_{n+1} - w)$ .

## 4.26. The Bessel functions.

4.26.1. Bessel function  $J_n(z)$  of first kind. The Bessel function  $J_n(z)$  of first kind and integer order n is defined as follows [1, Eq. (9.1.10)]:

(7) 
$$J_n(z) = (z/2)^n \sum_{k=0}^{\infty} \frac{(-z^2/4)^k}{k!(k+n)!}.$$

It is real for all real z, tends to 0 by oscillating around 0 when  $z \to \pm \infty$ , and tends to 0 when  $z \to 0$ , except  $J_0$  which tends to 1.

We use the following algorithm, with working precision w, and rounding to nearest:

```
x \leftarrow \circ(z^n)

y \leftarrow \circ(z^2)/4 [division by 4 is exact]

u \leftarrow \circ(n!)

t \leftarrow \circ(x/u)/2^n [division by 2^n is exact]

s \leftarrow t

for k from 1 do

t \leftarrow - \circ(ty)

t \leftarrow \circ(t/k)

t \leftarrow \circ(t/(k+n))

s \leftarrow \circ(s+t)

if |t| < \text{ulp}(s) and z^2 \le 2k(k+n) then return s.
```

The condition  $z^2 \leq 2k(k+n)$  ensures that the next term of the expansion is smaller than |t|/2, thus the sum of the remaining terms is smaller than |t| < ulp(s). Using Higham's method, with  $\theta$  denoting a random variable of value  $|\theta| \leq 2^{-w}$  — different instances of  $\theta$  denoting different values — we can write  $x = z^n(1+\theta)$ ,  $y = z^2/4(1+\theta)$ , and before the for-loop  $s = t = (z/2)^n/n!(1+\theta)^3$ . Now write  $t = (z/2)^n(-z^2/4)^k/(k!(k+n)!)(1+\theta)^{e_k}$  at the end of the for-loop with index k; each loop involves a factor  $(1+\theta)^4$ , thus we have  $e_k = 4k + 3$ . Now let T be an upper bound on the values of |t| and |s| during the for-loop, and assume we exit at k = K. The roundoff error in the additions  $\circ(s+t)$ , including the

error in the series truncation, is bounded by (K/2+1)ulp(T). The error in the value of t at step k is bounded by  $\epsilon_k := T|(1+\theta)^{4k+3}-1|$ ; if we assume  $(4k+3)2^{-w} \le 1/2$ , Lemma 2 yields  $\epsilon_k \le 2T(4k+3)2^{-w}$ . Summing from k=0 to K, this gives an absolute error bound on s at the end of the for-loop of:

$$(K/2+1)\text{ulp}(T) + 2(2K^2+5K+3)2^{-w}T \le (4K^2+21/2K+7)\text{ulp}(T),$$

where we used  $2^{-w}T \leq \text{ulp}(T)$ .

Large index n. For large index n, formula 9.1.62 from [1] gives  $|J_n(z)| \leq |z/2|^n/n!$ . Together with  $n! \geq \sqrt{2\pi n} (n/e)^n$ , which follows from example from [1, Eq. 6.1.38], this gives:

$$|J_n(z)| \le \frac{1}{\sqrt{2\pi n}} \left(\frac{ze}{2n}\right)^n.$$

Large argument. For large argument z, formula (7) requires at least  $k \approx z/2$  terms before starting to converge. If  $k \le z/2$ , it is better to use formula 9.2.5 from [1], which provides at least 2 bits per term:

$$J_n(z) = \sqrt{\frac{2}{\pi z}} [P(n, z) \cos \chi - Q(n, z) \sin \chi],$$

where  $\chi = z - (n/2 + 1/4)\pi$ , and P(n, z) and Q(n, z) are two diverging series:

$$P(n,z) \approx \sum_{k=0}^{\infty} (-1)^k \frac{\Gamma(1/2+n+2k)(2z)^{-2k}}{(2k)!\Gamma(1/2+n-2k)}, \quad Q(n,z) \approx \sum_{k=0}^{\infty} (-1)^k \frac{\Gamma(1/2+n+2k+1)(2z)^{-2k-1}}{(2k+1)!\Gamma(1/2+n-2k-1)}.$$

If n is real and non-negative — which is the case here —, the remainder of P(n, z) after k terms does not exceed the (k + 1)th term and is of the same sign, provided k > n/2 - 1/4; the same holds for Q(n, z) as long as k > n/2 - 3/4 [1, 9.2.10].

If we first approximate  $\chi = z - (n/2 + 1/4)\pi$  with working precision w, and then approximate  $\cos \chi$  and  $\sin \chi$ , there will be a huge relative error if  $z > 2^w$ . Instead, we use the fact that for n even,

$$P(n,z)\cos \chi - Q(n,z)\sin \chi = \frac{1}{\sqrt{2}}(-1)^{n/2}[P(\sin z + \cos z) + Q(\cos z - \sin z)],$$

and for n odd,

$$P(n,z)\cos \chi - Q(n,z)\sin \chi = \frac{1}{\sqrt{2}}(-1)^{(n-1)/2}[P(\sin z - \cos z) + Q(\cos z + \sin z)],$$

where  $\cos z$  and  $\sin z$  are computed accurately with  $mpfr\_sin\_cos$ , which uses in turn  $mpfr\_remainder$ .

If we consider P(n,z) and Q(n,z) together as one single series, its term of index k behaves like  $\Gamma(1/2+n+k)/k!/\Gamma(1/2+n-k)/(2z)^k$ . The ratio between the term of index k+1 and that of index k is about k/(2z), thus starts to diverge when  $k \approx 2z$ . At that point, the kth term is  $\approx e^{-2z}$ , thus if  $z > p/2 \log 2$ , we can use the asymptotic expansion.

4.26.2. Bessel function  $Y_n(z)$  of second kind. Like  $J_n(z)$ ,  $Y_n(z)$  is a solution of the linear differential equation:

$$z^{2}y'' + zy' + (z^{2} - n^{2})y = 0.$$

We have  $Y_{-n}(z) = (-1)^n Y_n(z)$  according to [1, Eq. (9.1.5)]; we now assume  $n \ge 0$ . When  $z \to 0^+$ ,  $Y_n(z)$  tends to  $-\infty$ ; when  $z \to +\infty$ ,  $Y_n(z)$  tends to 0 by oscillating around 0 like  $J_n(z)$ . We deduce from [23, Eq. (9.23)]:

$$Y_n(-z) = (-1)^n [Y_n(z) + 2iJ_n(z)],$$

which shows that for z > 0,  $Y_n(-z)$  is real only when z is a zero of  $J_n(z)$ ; assuming those zeroes are irrational,  $Y_n(z)$  is thus NaN for z negative.

Formula 9.1.11 from [1] gives:

$$Y_n(z) = -\frac{(z/2)^{-n}}{\pi} \sum_{k=0}^{n-1} \frac{(n-k-1)!}{k!} (z^2/4)^k + \frac{2}{\pi} \log(z/2) J_n(z)$$
$$- \frac{(z/2)^n}{\pi} \sum_{k=0}^{\infty} (\psi(k+1) + \psi(n+k+1)) \frac{(-z^2/4)^k}{k!(n+k)!},$$

where  $\psi(1) = -\gamma$ ,  $\gamma$  being Euler's constant (see §5.2), and  $\psi(n+1) = \psi(n) + 1/n$  for  $n \ge 1$ . Rewriting the above equation, we get

$$\pi Y_n(z) = -(z/2)^{-n} S_1 + S_2 - (z/2)^n S_3,$$

where  $S_1 = \sum_{k=0}^{n-1} \frac{(n-k-1)!}{k!} (z^2/4)^k$  is a finite sum,  $S_2 = 2(\log(z/2) + \gamma) J_n(z)$ , and  $S_3 = \sum_{k=0}^{\infty} (h_k + h_{n+k}) \frac{(-z^2/4)^k}{k!(n+k)!}$ , where  $h_k = 1 + 1/2 + \cdots + 1/k$  is the kth harmonic number. Once we have estimated  $-(z/2)^{-n} S_1 + S_2$ , we know to which relative precision we need to estimate the infinite sum  $S_3$ . For example, if  $(z/2)^n$  is small, typically a small relative precision on  $S_3$  will be enough.

We use the following algorithm to estimate  $S_1$ , with working precision w and rounding to nearest:

```
y \leftarrow \circ(z^2)/4 [division by 4 is exact]

f \leftarrow 1 [as an exact integer]

s \leftarrow 1

for k from n-1 downto 0 do

s \leftarrow \circ(ys)

f \leftarrow (n-k)(k+1)f [n!(n-k)!k! as exact integer]

s \leftarrow \circ(s+f)

f \leftarrow \sqrt{f} [integer, exact]

s \leftarrow \circ(s/f)
```

Let  $(1+\theta)^{\epsilon_j}-1$  be the maximum relative error on s after the look for  $k=n-j, 1 \leq j \leq n$ , i.e., the computed value is  $s_k(1+\theta)^{\epsilon_j}$  where  $s_k$  would be the value computed with no roundoff error, and  $|\theta| \leq 2^{-w}$ . Before the loop we have  $\epsilon_0 = 0$ . After the instruction  $s \leftarrow \circ(ys)$  the relative error can be written  $(1+\theta)^{\epsilon_{j-1}+2}-1$ , since  $y=z^2/4(1+\theta')$  with  $|\theta'| \leq 2^{-w}$ , and the product involves another rounding error. Since f is exact, the absolute error after  $s \leftarrow \circ(s+f)$  can be written  $|s_{\max}||(1+\theta)^{\epsilon_{j-1}+3}-1|$ , where  $|s_{\max}|$  is a bound for all computed values of s during the loop. The absolute error at the end of the for-loop can thus be written  $|s_{\max}||(1+\theta)^{3n}-1|$ , and  $|s_{\max}||(1+\theta)^{3n+1}-1|$  after the instruction  $s \leftarrow \circ(s/f)$ . If  $(3n+1)2^{-w} \leq 1/2$ , then using Lemma 2,  $|(1+\theta)^{3n+1}-1| \leq 2(3n+1)2^{-w}$ . Let e be the exponent difference between the maximum value of |s| during the for-loop and the final

value of s, then the relative error on the final s is bounded by

$$(3n+1)2^{e+1-w}$$
.

Assuming we compute  $(z/2)^n$  with correct rounding — using for example the mpfr\_pow\_ui function — and divide  $S_1$  by this approximation, the relative error on  $(z/2)^{-n}S_1$  will be at most  $(3n+3)2^{e+1-w}$ .

The computation of  $S_2$  is easier, still with working precision w and rounding to nearest:

```
t \leftarrow \circ(\log(z/2))
u \leftarrow \circ(\gamma)
v \leftarrow 2 \circ (t+u) \qquad \text{[multiplication by 2 is exact]}
x \leftarrow \circ(J_n(z))
s \leftarrow \circ(vx)
```

Since z/2 is exact, the error on t and u is at most one ulp, thus from §2.3 the ulp-error on v is at most  $1/2 + 2^{\exp(t) - \exp(v)} + 2^{\exp(u) - \exp(v)} \le 1/2 + 2^{e+1}$ , where  $e = \max(\exp(t), \exp(u)) - \exp(v)$ . Assuming e + 2 < w, then  $1/2 + 2^{e+1} \le 2^{w-1}$ , thus the total error on v is bounded by |v|, thus we can take  $c^+ = 2$  for v in the product  $s \leftarrow \circ(vx)$  (cf §2.4); similarly  $c^+ = 2$  applies to  $x \leftarrow \circ(J_n(z))$ , thus §2.4 yields the following bound for the ulp-error on s:

$$1/2 + 3(1/2 + 2^{e+1}) + 3(1/2) = 7/2 + 3 \cdot 2^{e+1} \le 2^{e+4}.$$

(Indeed, the smallest possible value of e is -1.)

The computation of  $S_3$  mimics that of  $J_n(z)$ . The only difference is that we have to compute the extra term  $h_k + h_{n+k}$ , that we maintain as an exact rational p/q, p and q being integers:

```
x \leftarrow \circ(z^n)
y \leftarrow \circ(z^2)/4 [division by 4 is exact]
u \leftarrow \circ(n!)
t \leftarrow \circ(x/u)/2^n [division by 2^n is exact]
p/q \leftarrow h_n
                       [exact rational]
u \leftarrow \circ (pt)
s \leftarrow \circ (u/q)
for k from 1 do
    t \leftarrow - \circ (ty)
    t \leftarrow \circ (t/k)
    t \leftarrow \circ (t/(k+n))
    p/q \leftarrow p/q + 1/k + 1/(n+k)
                                                           [exact]
    u \leftarrow \circ (pt)
    u \leftarrow \circ (u/q)
    s \leftarrow \circ (s+u)
    if |u| < \text{ulp}(s) and z^2 \le 2k(k+n) then return s.
```

Using  $(h_{k+1} + h_{n+k+1})k \leq (h_k + h_{n+k})(k+1)$ , which is true for  $k \geq 1$  and  $n \geq 0$ , the condition  $z^2 \leq 2k(k+n)$  ensures that the next term of the expansion is smaller than |t|/2, thus the sum of the remaining terms is smaller than |t| < ulp(s). The difference with the error analysis of  $J_n$  is that here  $e_k = 6k + 5$  instead of  $e_k = 4k + 3$ . Denote U an upper bound on the values of u, s during the for-loop — note that  $|u| \geq |t|$  by construction — and assume we

exit at k = K. The error in the value of u at step k is bounded by  $\epsilon_k := U[(1+\theta)^{6k+5} - 1];$ Assuming  $(6k+5)2^{-w} \le 1/2$ , Lemma 2 yields  $\epsilon_k \le 2U(6k+5)2^{-w}$ , and the sum from k=0to K gives an absolute error bound on s at the end of the for-loop bounded by:

$$(K/2+1)\text{ulp}(U) + 2(3K^2+8K+5)2^{-w}U \le (6K^2+33/2K+11)\text{ulp}(U),$$

where we used  $2^{-w}U \leq \text{ulp}(U)$ .

4.27. The Dilogarithm function. The mpfr\_li2 function computes the real part of the dilogarithm function defined by:

$$\operatorname{Li}_{2}(x) = -\int_{0}^{x} \frac{\log(1-t)}{t} dt.$$

The above relation defines a multivalued function in the complex plane, we choose a branch so that  $\text{Li}_2(x)$  is real for x real, x < 1 and we compute only the real part for x real,  $x \ge 1$ . When  $x \in ]0, \frac{1}{2}]$ , we use the series (see [24, Eq. (5)]):

$$\operatorname{Li}_{2}(x) = \sum_{n=0}^{\infty} \frac{B_{n}}{(n+1)!} (-\log(1-x))^{n+1}$$

where  $B_n$  is the *n*-th Bernoulli number.

Otherwise, we perform an argument reduction using the following identities (see [8]):

Otherwise, we perform an argument reduction using the following identities (see [8]): 
$$x \in [2, +\infty[$$
  $\Re(\text{Li}_2(x)) = \frac{\pi^2}{3} - \frac{1}{2}\log^2(x) - \text{Li}_2\left(\frac{1}{x}\right)$   $x \in ]1, 2[$   $\Re(\text{Li}_2(x)) = \frac{\pi^2}{6} - \log(x)\left[\log(x-1) - \frac{1}{2}\log(x)\right] + \text{Li}_2\left(1 - \frac{1}{x}\right)$   $\text{Li}_2(1) = \frac{\pi^2}{6}$   $x \in ]\frac{1}{2}, 1[$   $\text{Li}_2(x) = \frac{\pi^2}{6} - \log(x)\log(1-x) - \text{Li}_2(1-x)$   $\text{Li}_2(0) = 0$   $x \in [-1, 0[$   $\text{Li}_2(x) = -\frac{1}{2}\log^2(1-x) - \text{Li}_2\left(\frac{x}{x-1}\right)$   $x \in ]-\infty, -1[$   $\text{Li}_2(x) = -\frac{\pi^2}{6} - \frac{1}{2}\log(1-x)[2\log(-x) - \log(1-x)] + \text{Li}_2\left(\frac{1}{1-x}\right)$ . Assume first  $0 < x \le \frac{1}{2}$ , the odd Bernoulli numbers being zero (except  $B_1 = -\frac{1}{2}$ ), we can

rewrite  $\text{Li}_2(x)$  in the form:

$$Li_2(x) = -\frac{\log^2(1-x)}{4} + S(-\log(1-x))$$

where

$$S(z) = \sum_{k=0}^{\infty} \frac{B_{2k}}{(2k+1)!} z^{2k+1}.$$

Let  $S_N(z) = \sum_{k \leq N} \frac{B_{2k}}{(2k+1)!} z^{2k+1}$  the N-th partial sum, and  $R_N(z)$  the truncation error. The even Bernoulli numbers verify the following inequality for all  $n \ge 1$  ([1, Inequalities 23.1.15]):

$$\frac{2(2n)!}{(2\pi)^{2n}} < |B_{2n}| < \frac{2(2n)!}{(2\pi)^{2n}} \left(\frac{1}{1 - 2^{1 - 2n}}\right),$$

so we have for all  $N \geq 0$ 

$$\frac{|B_{2N+2}|}{(2N+3)!}|z|^{2N+3} < \frac{2|z|}{(1-2^{-2N-1})(2N+3)} \left| \frac{z}{2\pi} \right|^{2N+2},$$

showing that S(z) converges for  $|z| < 2\pi$ . As the series is alternating, we then have an upper bound for the truncation error  $|R_N(z)|$  when  $0 < z \le \log 2$ :

$$|R_N(z)| < 2^{\exp(z) - 6N - 5}$$
.

The partial sum  $S_N(z)$  computation is implemented as follows:

```
Algorithm 1i2_series
```

Input: z with  $z \in ]0, \log 2]$ 

Output:  $\circ(S(z))$ 

 $u \leftarrow \triangle(z^2)$ 

 $v \leftarrow \triangle(z)$ 

 $s \leftarrow \triangle(z)$ 

## for k from 1 do

 $v \leftarrow \triangle(uv)$ 

 $v \leftarrow \triangle(v/(2k))$ 

 $v \leftarrow \triangle(v/(2k))$ 

 $v \leftarrow \triangle(v/(2k+1))$ 

 $v \leftarrow \triangle(v/(2k+1))$ 

 $w \leftarrow \mathcal{N}(vB'_k)$ 

 $s \leftarrow \mathcal{N}(s+w)$ 

if |w| < ulp(s) then return s.

where  $B'_k = B_{2k}(2k+1)!$  is an exact representation in mpn integers.

Let p the working precision. Using Higham's method, before entering the loop we have  $u=z^2(1+\theta), v=s=z(1+\theta)$  where different instances of  $\theta$  denote different variables and  $|\theta| \le 2^{-p}$ . After the k-th loop,  $v = z^{2k+1}/((2k+1)!2k(2k+1))(1+\theta)^{6k}$ ,  $w = B_{2k}z^{2k+1}/(2k+1)$ 1)! $(1+\theta)^{6k+1}$ .

When  $x \in ]0, \frac{1}{2}]$ , Li<sub>2</sub>(x) calculation is implemented as follows

Algorithm  $1i2_0..+\frac{1}{2}$ 

Input: x with  $x \in \left]0, \frac{1}{2}\right]$ , the output precision n, and a rounding mode  $\circ_n$ 

Output:  $\circ_n(\text{Li}_2(x))$ 

$$u \leftarrow \mathcal{N}(1-x)$$
 error(u)  $\leq \frac{1}{2} \text{ulp}(u)$ 

$$\begin{array}{lll} u \leftarrow \mathcal{N}(1-x) & \operatorname{error}(u) & \leq & \frac{1}{2}\mathrm{ulp}(u) \\ u \leftarrow \triangle(-\log(u)) & \operatorname{error}(u) & \leq & (1+2^{-\operatorname{Exp}(u)})\mathrm{ulp}(u) \\ t \leftarrow \triangle(S(u)) & \operatorname{error}(t) & \leq & (k+1)2^{1-\operatorname{Exp}(t)}\mathrm{ulp}(t) \end{array}$$

$$t \leftarrow \triangle(S(u))$$
 error $(t) \leq (k+1)2^{1-\exp(t)} \operatorname{ulp}(t)$ 

$$v \leftarrow \triangle(u^2)$$

$$v \leftarrow \triangle(v/4)$$
 error $(v) \le (5 + 2^{2 - \exp(u)}) \operatorname{ulp}(v)$ 

$$s \leftarrow \mathcal{N}(t - v)$$
  $error(s) \le 2^{\kappa_s} \text{ulp}(s)$ 

if s cannot be exactly rounded according to the given mode  $\circ_n$ 

then increase the working precision and restart calculation

else return  $\circ_n(s)$ 

where 
$$\kappa_s = \max(-1, \lceil \log_2(k+1) \rceil + 1 - \exp(s), \max(1, -\exp(u)) - 1 - \exp(s))$$

When x is large and positive, we can use an asymptotic expansion near  $+\infty$  using the fact that  $\operatorname{Li}_2\left(\frac{1}{x}\right) = \frac{1}{x} + O\left(\frac{1}{x^2}\right)$  (see below):

$$\left| \text{Li}_2(x) + \frac{\log^2 x}{2} - \frac{\pi^2}{3} \right| \le \frac{2}{x}$$

which gives the following algorithm:

Algorithm li2\_asympt\_pos

Input: x with  $x \geq 38$ , the output precision n, and a rounding mode  $\circ_n$ Output:  $\circ_n(\Re(\text{Li}_2(x)))$  if it can round exactly, a failure indicator if not

 $u \leftarrow \mathcal{N}(\log x)$ 

 $v \leftarrow \mathcal{N}(u^2)$ 

 $g \leftarrow \mathcal{N}(v/2)$ 

 $p \leftarrow \mathcal{N}(\pi)$ 

 $q \leftarrow \mathcal{N}(p^2)$ 

 $h \leftarrow \mathcal{N}(q/3)$ 

 $s \leftarrow \mathcal{N}(q-h)$ 

if s cannot be exactly rounded according to the given mode  $\circ_n$ 

then return failed

else return  $\circ_p(n)$ 

Else, if  $x \in [2,38]$  or if  $x \ge 38$  but the above calculation cannot give exact rounding, we use the relation

$$\operatorname{Li}_{2}(x) = -S\left(-\log(1-\frac{1}{x})\right) + \frac{\log^{2}\left(1-\frac{1}{x}\right)}{4} - \frac{\log^{2}x}{2} + \frac{\pi^{2}}{3},$$

which is computed as follows:

Algorithm  $1i2_2..+\infty$ 

Input: x with  $x \in [2, +\infty[$ , the output precision n, and a rounding mode  $\circ_n$ 

Output:  $\circ_n(\Re(\text{Li}_2(x)))$ 

$$y \leftarrow \mathcal{N}(-1/x)$$
 error $(y) \leq \frac{1}{2} \text{ulp}(y)$ 

$$y \leftarrow \mathcal{N}(-1/x)$$
  $\operatorname{error}(y) \leq \frac{1}{2}\operatorname{ulp}(y)$   
 $u \leftarrow \triangle(-\log(1+y))$   $\operatorname{error}(u) \leq (1+2^{1-\operatorname{Exp}(u)})\operatorname{ulp}(u)$ 

$$q \leftarrow \mathcal{N}(-S(u))$$
 error $(q) \leq 2(k+1)2^{-\exp(q)} \text{ulp}(q)$ 

 $v \leftarrow \triangle(u^2)$ 

$$v \leftarrow \triangle(v/4)$$
 error $(v) \leq (5 + 2^{3 - \exp(u)}) \operatorname{ulp}(v)$   
 $r \leftarrow \mathcal{N}(q + v)$  error $(r) \leq 2^{\kappa_r} \operatorname{ulp}(r)$ 

$$r \leftarrow \mathcal{N}(q+v)$$
 error $(r) \leq 2^{\kappa_r} \text{ulp}(r)$ 

 $w \leftarrow \triangle(\log x)$ 

 $w \leftarrow \mathcal{N}(w^2)$ 

$$w \leftarrow \mathcal{N}(w/2)$$
 error $(w) \leq \frac{9}{2} \text{ulp}(w)$   
 $s \leftarrow \mathcal{N}(r-w)$  error $(s) \leq 2^{\kappa_s} \text{ulp}(s)$ 

$$s \leftarrow \mathcal{N}(r - w)$$
  $\operatorname{error}(s) \leq \tilde{2}^{\kappa_s} \operatorname{ulp}(s)$ 

 $p \leftarrow \triangle(\pi)$ 

 $p \leftarrow \mathcal{N}(p^2)$ 

$$p \leftarrow \mathcal{N}(p)$$

$$p \leftarrow \mathcal{N}(p/3) \qquad \text{error}(p) \leq \frac{19}{2} \text{ulp}(p) \leq 2^{2-\text{Exp}(p)} \text{ulp}(p)$$

$$t \leftarrow \mathcal{N}(s+p) \qquad \text{error}(t) \leq 2^{\kappa_t} \text{ulp}(t)$$

if t can be exactly rounded according to  $\circ_n$ 

then return  $\circ_n(t)$ 

else increase working precision and restart calculation

with

$$\kappa_r = 2 + \max(-1, \lceil \log_2(k+1) \rceil + 1 - \exp(r), 3 + \max(1, -\exp(u)) + \exp(v) - \exp(r))$$

$$\kappa_s = 2 + \max(-1, \kappa_r + \exp(r) - \exp(s), 3 + \exp(w) - \exp(s))$$

$$\kappa_t = 2 + \max(-1, \kappa_s + \exp(s) - \exp(t), 2 - \exp(t))$$

When  $x \in ]1, 2[$ , we use the relation

$$\text{Li}_2(x) = S(\log x) + \frac{\log^2 x}{4} - \log x \log(x - 1) + \frac{\pi^2}{6}$$

which is implemented as follows

Algorithm 1i2\_1..2

Input: x with  $x \in ]1,2[$ , the output precision n, and a rounding mode  $\circ_n$ 

Output:  $\circ_n(\Re(\text{Li}_2(x)))$ 

$$\begin{array}{lll} l \leftarrow \triangle(\log x) & \operatorname{error}(l) & \leq & \operatorname{ulp}(l) \\ q \leftarrow \mathcal{N}(S(l)) & \operatorname{error}(q) & \leq & (k+1)2^{1-\operatorname{Exp}(q)} \operatorname{ulp}(q) \\ u \leftarrow \mathcal{N}(l^2) & & & \\ u \leftarrow \mathcal{N}(u/4) & \operatorname{error}(u) & \leq & \frac{5}{2} \operatorname{ulp}(u) \\ r \leftarrow \mathcal{N}(q+u) & \operatorname{error}(r) & \leq & (3+(k+1)2^{1-\operatorname{Exp}(q)}) \operatorname{ulp}(r) \\ y \leftarrow \mathcal{N}(x-1) & \operatorname{error}(y) & \leq & \frac{1}{2} \operatorname{ulp}(y) \\ v \leftarrow \triangle(\log y) & \operatorname{error}(v) & \leq & (1+2^{-\operatorname{Exp}(v)}) \operatorname{ulp}(v) \\ w \leftarrow \mathcal{N}(ul) & \operatorname{error}(w) & \leq & (\frac{15}{2}+2^{1-\operatorname{Exp}(v)}) \operatorname{ulp}(w) \\ s \leftarrow \mathcal{N}(r-w) & \operatorname{error}(s) & \leq & (11+(k+1)2^{1-\operatorname{Exp}(q)}+2^{1-\operatorname{Exp}(v)}) \operatorname{ulp}(s) \\ p \leftarrow \triangle(\pi) \\ p \leftarrow \mathcal{N}(p^2) \\ p \leftarrow \mathcal{N}(p/6) & \operatorname{error}(p) & \leq & \frac{19}{2} \operatorname{ulp}(p) \end{array}$$

 $\operatorname{error}(p) \leq \frac{19}{2} \operatorname{ulp}(p)$   $\operatorname{error}(t) \leq (31 + (k+1)2^{1-\operatorname{Exp}(q)} + 2^{1-\operatorname{Exp}(v)}) \operatorname{ulp}(t)$  $t \leftarrow \mathcal{N}(s+p)$ 

if t can be exactly rounded according to  $\circ_n$ 

then return  $\circ_n(t)$ 

else increase working precision and restart calculation

we use the fact that  $S(\log x) \ge 0$  and  $u \ge 0$  for  $\operatorname{error}(r)$ , that  $r \ge 0$  and  $-\log x \log(x-1) \ge 0$ 0 for error(s), and that  $s \ge 0$  for error(t).

When x=1, we have a simpler value  $\text{Li}_2(1)=\frac{\pi^2}{6}$  whose computation is implemented as follows

Algorithm 1i2\_1

Input: the output precision p, and a rounding mode  $\circ_p$ 

Output:  $\circ_p(\frac{\pi^2}{6})$ 

$$u \leftarrow \triangle(\pi)$$

$$u \leftarrow \mathcal{N}(u^2)$$

$$u \leftarrow \mathcal{N}(u/6) \quad \text{error}(u) \leq \frac{19}{2} \text{ulp}(u)$$

 $u \leftarrow \mathcal{N}(u/6) \quad \text{error}(u) \leq \frac{19}{2} \text{ulp}(u)$ if u can be exactly rounded according to  $\circ_p$ 

then return  $\circ_p(u)$ 

else increase working precision and restart calculation

When  $x \in \frac{1}{2}, 1$ , we use the relation

$$Li_2(x) = -S(-\log x) - \log x \log(1-x) + \frac{\log^2 x}{4} + \frac{\pi^2}{6}$$

which is implemented as follows

Algorithm li2\_0.5..1

Input: x with  $x \in \left[\frac{1}{2}, 1\right]$ , the output precision n, and a rounding mode  $\circ_n$ 

Output:  $\circ_n(Li2(x))$ 

$$\begin{array}{lll} l \leftarrow \triangle(-\log x) & \operatorname{error}(l) & \leq & \operatorname{ulp}(l) \\ q \leftarrow \mathcal{N}(-S(l)) & \operatorname{error}(q) & \leq & (k+1)2^{1-\operatorname{Exp}(q)}\operatorname{ulp}(q) \\ y \leftarrow \mathcal{N}(1-x) & \operatorname{error}(y) & \leq & \frac{1}{2}\operatorname{ulp}(y) \\ u \leftarrow \triangle(\log y) & \operatorname{error}(u) & \leq & (1+2^{-\operatorname{Exp}(v)})\operatorname{ulp}(u) \\ v \leftarrow \mathcal{N}(ul) & \operatorname{error}(v) & \leq & (\frac{9}{2}+2^{1-\operatorname{Exp}(v)})\operatorname{ulp}(v) \\ r \leftarrow \mathcal{N}(q+v) & \operatorname{error}(r) & \leq & 2^{\kappa_r}\operatorname{ulp}(r) \\ w \leftarrow \mathcal{N}(l^2) & \\ w \leftarrow \mathcal{N}(u/4) & \operatorname{error}(w) & \leq & \frac{5}{2}\operatorname{ulp}(w) \\ s \leftarrow \mathcal{N}(r+w) & \operatorname{error}(s) & \leq & 2^{\kappa_s}\operatorname{ulp}(s) \\ p \leftarrow \triangle(\pi) & \\ p \leftarrow \mathcal{N}(p^2) & \\ p \leftarrow \mathcal{N}(p/6) & \operatorname{error}(p) & \leq & \frac{19}{2}\operatorname{ulp}(p) \leq 2^{3-\operatorname{Exp}(p)}\operatorname{ulp}(p) \\ t \leftarrow \mathcal{N}(s+p) & \operatorname{error}(t) & \leq & 2^{\kappa_t}\operatorname{ulp}(t) \\ \text{if } t \text{ can be exactly rounded according to } \circ_n \end{array}$$

then return  $\circ_n(t)$ 

else increase working precision and restart calculation

where

$$\kappa_r = 2 + \max(3, \lceil \log_2(k+1) \rceil + 1 - \exp(q), 1 - \exp(u))$$

$$\kappa_s = 2 + \max(-1, \kappa_r + \exp(r) - \exp(s), 2 + \exp(w) - \exp(s))$$

$$\kappa_t = 2 + \max(-1, \kappa_s + \exp(s) - \exp(t), 3 - \exp(t))$$

Near 0, we can use the relation

$$\operatorname{Li}_2(x) = \sum_{n=0}^{\infty} \frac{x^k}{k^2}$$

which is true for  $|x| \leq 1$  [FIXME: ref]. If  $x \leq 0$ , we have  $0 \leq \text{Li}_2(x) - x \leq \frac{x^2}{4}$  and if x is positive,  $0 \le \text{Li}_2(x) - x \le (\frac{\pi^2}{6} - 1)x^2 \le x^2 \le 2^{2\exp(x) + 1} \text{ulp}(x)$ . When  $x \in [-1, 0[$ , we use the relation

$$\text{Li}_2(x) = -S(-\log(1-x)) - \frac{\log^2(1-x)}{4}$$

which is implemented as follows

Algorithm 1i2\_-1..0

Input: x with  $x \in ]-1,0[$ , the output precision n, and a rounding mode  $\circ_n$ 

Output:  $\circ_n(Li2(x))$ 

$$y \leftarrow \mathcal{N}(1-x) \qquad \text{error}(y) \leq \frac{1}{2} \text{ulp}(y)$$

$$l \leftarrow \Delta(\log y) \qquad \text{error}(l) \leq (1+2^{-\exp(l)}) \text{ulp}(l)$$

$$r \leftarrow \mathcal{N}(-S(l)) \qquad \text{error}(r) \leq (k+1)2^{1-\exp(r)} \text{ulp}(r)$$

$$u \leftarrow \mathcal{N}(-l^2)$$

$$u \leftarrow \mathcal{N}(u/4) \qquad \text{error}(u) \leq (\frac{9}{2}+2^{-\exp(l)}) \text{ulp}(u)$$

$$s \leftarrow \mathcal{N}(r+u) \qquad \text{error}(s) \leq 2^{\kappa_s} \text{ulp}(s)$$

if s can be exactly rounded according to  $\circ_n$ 

then return  $\circ_n(s)$ 

else increase working precision and restart calculation

with

$$\kappa_s = 2 + \max(3, \lceil \log_2(k+1) \rceil + 1 - \exp(r), -\exp(l))$$

When x is large and negative, we can use an asymptotic expansion near  $-\infty$ :

$$\left| \operatorname{Li}_2(x) + \frac{\log^2(-x)}{2} + \frac{\pi^2}{3} \right| \le \frac{1}{|x|}$$

which gives the following algorithm:

Algorithm li2\_asympt\_neg

Input: x with  $x \leq -7$ , the output precision n, and a rounding mode  $\circ_n$  Output:  $\circ_n(\text{Li}_2(x))$  if it can round exactly, a failure indicator if not

 $l \leftarrow \mathcal{N}(\log(-x))$ 

 $f \leftarrow \mathcal{N}(l^2)$ 

 $g \leftarrow \mathcal{N}(f/2)$ 

 $p \leftarrow \mathcal{N}(\pi)$ 

 $q \leftarrow \mathcal{N}(p^2)$ 

 $h \leftarrow \mathcal{N}(q/3)$ 

 $s \leftarrow \mathcal{N}(g-h)$ 

if s cannot be exactly rounded according to the given mode  $\circ_n$ 

then return failed

else return  $\circ_n(s)$ 

When  $x \in ]-7,-1[$  or if the above computation cannot give exact rounding, we use the relation

$$\operatorname{Li}_{2}(x) = S\left(\log\left(1 - \frac{1}{x}\right)\right) - \frac{\log^{2}(-x)}{4} - \frac{\log(-x)\log(1 - x)}{2} + \frac{\log^{2}(1 - x)}{4} + \frac{\pi^{2}}{6}$$

which is implemented as follows

Algorithm  $1i2_{-}\infty..-1$ 

Input: x with  $x \in ]-\infty, -1[$ , the output precision n, and a rounding mode  $\circ_n$ 

Output:  $\circ_n(\text{Li}_2(x))$ 

$$\begin{array}{llll} y \leftarrow \mathcal{N}(-1/x) \\ z \leftarrow \mathcal{N}(1+y) \\ z \leftarrow \mathcal{N}(\log z) \\ o \leftarrow \mathcal{N}(S(z)) & \operatorname{error}(o) & \leq (k+1)2^{1-\operatorname{exp}(o)} \operatorname{ulp}(o) \\ y \leftarrow \mathcal{N}(1-x) \\ u \leftarrow \triangle(\log y) & \operatorname{error}(u) & \leq (1+2^{-\operatorname{exp}(u)}) \operatorname{ulp}(u) \\ v \leftarrow \triangle(\log(-x)) & \operatorname{error}(v) & \leq \operatorname{ulp}(v) \\ w \leftarrow \mathcal{N}(uv) \\ w \leftarrow \mathcal{N}(w/2) & \operatorname{error}(w) & \leq (\frac{9}{2}+1) \operatorname{ulp}(w) \\ q \leftarrow \mathcal{N}(o-w) & \operatorname{error}(q) & \leq 2^{\kappa_q} \operatorname{ulp}(q) \\ v \leftarrow \mathcal{N}(v/2) & \operatorname{error}(v) & \leq \frac{9}{2} \operatorname{ulp}(v) \\ r \leftarrow \mathcal{N}(q-v) & \operatorname{error}(r) & \leq 2^{\kappa_r} \operatorname{ulp}(r) \\ w \leftarrow \mathcal{N}(u^2) & w \leftarrow \mathcal{N}(w/4) & \operatorname{error}(w) & \leq \frac{17}{2} \operatorname{ulp}(w) \\ s \leftarrow \mathcal{N}(r+w) & \operatorname{error}(s) & \leq 2^{\kappa_s} \operatorname{ulp}(s) \\ p \leftarrow \mathcal{N}(p) & & \operatorname{error}(p) & \leq \frac{19}{2} \operatorname{ulp}(p) \leq 2^{3-\operatorname{exp}(p)} \operatorname{ulp}(p) \\ t \leftarrow \mathcal{N}(s-p) & \operatorname{error}(t) & \leq 2^{\kappa_t} \operatorname{ulp}(t) \end{array}$$

if t can be exactly rounded according to  $\circ_n$ 

then return  $\circ_n(t)$ 

else increase working precision and restart calculation

where

$$\kappa_q = 1 + \max(3, \lceil \log_2(k+1) \rceil + 1 - \exp(q))$$

$$\kappa_r = 2 + \max(-1, \kappa_q + \exp(q) - \exp(r), 3 + \exp(v) - \exp(r))$$

$$\kappa_s = 2 + \max(-1, \kappa_r + \exp(r) - \exp(s), 3 + \exp(w) - \exp(s))$$

$$\kappa_t = 2 + \max(-1, \kappa_s + \exp(s) - \exp(t), 3 - \exp(t))$$

4.28. **Summary.** Table 1 presents the generic error for several operations, assuming all variables have a mantissa of p bits, and no overflow/underflow occurs. The inputs u and v are approximations of x and y with  $|u-x| \le k_u \text{ulp}(u)$  and  $|v-y| \le k_v \text{ulp}(v)$ . The additional rounding error  $c_w$  is 1/2 for rounding to nearest, and 1 otherwise. The value  $c_u^{\pm}$  equals  $1 \pm k_u 2^{1-p}$ .

Remark: in the addition case, when uv > 0, necessarily one of  $2^{e_u - e_w}$  and  $2^{e_v - e_w}$  is less than 1/2, thus  $\operatorname{err}(w)/\operatorname{ulp}(w) \leq c_w + \max(k_u + k_v/2, k_u/2 + k_v) \leq c_w + \frac{3}{2}\max(k_u, k_v)$ .

## 5. Mathematical constants

5.1. The constant  $\pi$ . The computation of  $\pi$  uses the AGM formula

$$\pi = \frac{\mu^2}{D},$$

where  $\mu = \text{AGM}(\frac{1}{\sqrt{2}}, 1)$  is the common limit of the sequences  $a_0 = 1, b_0 = \frac{1}{\sqrt{2}}, a_{k+1} = (a_k + b_k)/2, b_{k+1} = \sqrt{a_k b_k}, D = \frac{1}{4} - \sum_{k=1}^{\infty} 2^{k-1} (a_k^2 - b_k^2)$ . This formula can be evaluated

w	$\operatorname{err}(w)/\operatorname{ulp}(w) \le c_w + \dots$	special case
$\circ (u+v)$	$k_u 2^{e_u - e_w} + k_v 2^{e_v - e_w}$	$k_u + k_v$ if $uv \ge 0$
$\circ (u \cdot v)$	$(1+c_u^+)k_u + (1+c_v^+)k_v$	$2k_u + 2k_v$ if $u \ge x, v \ge y$
$\circ (1/v)$	$4k_v$	$2k_v$ if $v \leq y$
$\circ (u/v)$	$4k_u + 4k_v$	$2k_u + 2k_v$ if $v \le y$
$\circ(\sqrt{u})$	$2k_u/(1+\sqrt{c_u^-})$	$k_u$ if $u \leq x$
$\circ(e^u)$	$e^{k_u 2^{e_u - p}} 2^{e_u + 1} k_u$	$2^{e_u+1}k_u$ if $u \ge x$
$\circ(\log u)$	$k_u 2^{1-e_w}$	

Table 1. Generic error

efficiently as shown in [19], starting from  $a_0 = A_0 = 1$ ,  $B_0 = 1/2$ ,  $D_0 = 1/4$ , where  $A_k$  and  $B_k$  represent respectively  $a_k^2$  and  $b_k^2$ :

$$S_{k+1} \leftarrow (A_k + B_k)/4$$

$$b_k \leftarrow \sqrt{B_k}$$

$$a_{k+1} \leftarrow (a_k + b_k)/2$$

$$A_{k+1} \leftarrow a_k^2$$

$$B_{k+1} \leftarrow 2(A_{k+1} - S_{k+1})$$

$$D_{k+1} \leftarrow D_k - 2^k(A_{k+1} - B_{k+1})$$

For each variable x approximation a true value  $\tilde{x}$ , denote by  $\epsilon(x)$  the exponent of the maximal error, i.e.  $x = \tilde{x}(1 \pm \delta)^e$  with  $|e| \le \epsilon(x)$ , and  $\delta = 2^{-p}$  for precision p (we assume all roundings to nearest). We can prove by an easy induction that  $\epsilon(a_k) = 3 \cdot 2^{k-1} - 1$ , for  $k \ge 1$ ,  $\epsilon(A_k) = 3 \cdot 2^k - 1$ ,  $\epsilon(B_k) = 6 \cdot 2^k - 6$ . Thus the relative error on  $B_k$  is at most  $12 \cdot 2^{k-p}$ , — assuming  $12 \cdot 2^{k-p} \le 1$  — which is at most  $12 \cdot 2^k \text{ulp}(B_k)$ , since  $1/2 \le B_k$ .

If we stop when  $|A_k - B_k| \le 2^{k-p}$  where p is the working precision, then  $|\mu^2 - B_k| \le 13 \cdot 2^{k-p}$ . The error on D is bounded by  $\sum_{j=0}^k 2^j (6 \cdot 2^{k-p} + 12 \cdot 2^{k-p}) \le 6 \cdot 2^{2k-p+2}$ , which gives a relative error less than  $2^{2k-p+7}$  since  $D_k \ge 3/16$ .

Thus we have  $\pi = \frac{B_k(1+\epsilon)}{D(1+\epsilon')}$  with  $|\epsilon| \le 13 \cdot 2^{k-p}$  and  $|\epsilon'| \le 2^{2k-p+7}$ . This gives  $\pi = \frac{B_k}{D}(1+\epsilon'')$  with  $|\epsilon''| \le 2\epsilon + \epsilon' \le (26 + 2^{k+7})2^{k-p} \le 2^{2k-p+8}$ , assuming  $|\epsilon'| \le 1$ .

5.2. **Euler's constant.** Euler's constant is computed using the formula  $\gamma = S(n) - R(n) - \log n$  where:

$$S(n) = \sum_{k=1}^{\infty} \frac{n^k (-1)^{k-1}}{k! k}, \quad R(n) = \int_n^{\infty} \frac{\exp(-u)}{u} du \sim \frac{\exp(-n)}{n} \sum_{k=0}^{\infty} \frac{k!}{(-n)^k}.$$

This identity is attributed to Sweeney by Brent [4]. (See also [21].) We have  $S(n) =_2 F_2(1,1;2,2;-n)$  and R(n) = Ei(1,n).

EVALUATION OF S(n). As in [4], let  $\alpha \sim 4.319136566$  the positive root of  $\alpha + 2 = \alpha \log \alpha$ , and  $N = \lceil \alpha n \rceil$ . We approximate S(n) by

$$S'(n) = \sum_{k=1}^{N} \frac{n^k (-1)^{k-1}}{k!k}.$$

The remainder term S(n) - S'(n) is bounded by:

$$|S(n) - S'(n)| \le \sum_{k=N+1}^{\infty} \frac{n^k}{k!}.$$

Since  $k! \ge (k/e)^k$ , and  $k \ge N + 1 \ge \alpha n$ , we have:

$$|S(n) - S'(n)| \le \sum_{k=N+1}^{\infty} \left(\frac{ne}{k}\right)^k \le \sum_{k=N+1}^{\infty} \left(\frac{e}{\alpha}\right)^k \le 2\left(\frac{e}{\alpha}\right)^N \le 2e^{-2n}$$

since  $(e/\alpha)^{\alpha} = e^{-2}$ .

To approximate S'(n), we use the binary splitting method, which computes integers T and Q such that  $S'(n) = \frac{T}{Q}$  exactly, then we compute  $t = \circ(T)$ , and  $s = \circ(t/Q)$ , both with rounding to nearest. If the working precision is w, we have  $t = T(1+\theta_1)$  and  $s = t/Q(1+\theta_2)$  where  $|\theta_i| \leq 2^{-w}$ . If follows  $s = T/Q(1+\theta_1)(1+\theta_2)$ , thus the error on s is less than 3 ulps, since  $(1+2^{-w})^2 \leq 1+3\cdot 2^{-w}$ .

EVALUATION OF R(n). We estimate R(n) using the terms up to k = n - 2, again as in [4]:

$$R'(n) = \frac{e^{-n}}{n} \sum_{k=0}^{n-2} \frac{k!}{(-n)^k}.$$

Let us introduce  $I_k = \int_n^\infty \frac{e^{-u}}{u^k} du$ . We have  $R(n) = I_1$  and the recurrence  $I_k = \frac{e^{-n}}{n^k} - kI_{k+1}$ , which gives

$$R(n) = \frac{e^{-n}}{n} \sum_{k=0}^{n-2} \frac{k!}{(-n)^k} + (-1)^{n-1} (n-1)! I_n.$$

Bounding n! by  $(n/e)^n \sqrt{2\pi(n+1)}$  which holds<sup>3</sup> for  $n \ge 1$ , we have:

$$|R(n) - R'(n)| = (n-1)! I_n \le \frac{n!}{n} \int_n^\infty \frac{e^{-n}}{u^n} du \le \frac{n^{n-1}}{e^n} \sqrt{2\pi(n+1)} \frac{e^{-n}}{(n-1)n^{n-1}}$$

and since  $\sqrt{2\pi(n+1)}/(n-1) \le 1$  for  $n \ge 9$ :

$$|R(n) - R'(n)| \le e^{-2n} \quad \text{for } n \ge 9.$$

Thus we have:

$$|\gamma - S'(n) - R'(n) - \log n| \le 3e^{-2n}$$
 for  $n \ge 9$ .

To approximate R'(n), we use the following:

$$m \leftarrow \operatorname{prec}(x) - \lfloor \frac{n}{\log 2} \rfloor$$

$$a \leftarrow 2^{m}$$

$$s \leftarrow 1$$
**for**  $k$  **from** 1 **to**  $n$  **do**

$$a \leftarrow \lfloor \frac{ka}{n} \rfloor$$

$$s \leftarrow s + (-1)^{k}a$$

$$t \leftarrow \lfloor s/n \rfloor$$

$$x \leftarrow t/2^m$$
  
return  $r = e^{-n}x$ 

The absolute error  $\epsilon_k$  on a at step k satisfies  $\epsilon_k \leq 1 + k/n\epsilon_{k-1}$  with  $\epsilon_0 = 0$ . As  $k/n \leq 1$ , we have  $\epsilon_k \leq k$ , whence the error on s is bounded by n(n+1)/2, and that on t by  $1+(n+1)/2 \leq n+1$  since  $n \geq 1$ . The operation  $x \leftarrow t/2^m$  is exact as soon as  $\operatorname{prec}(x)$  is large enough, thus the error on x is at most  $(n+1)\frac{e^n}{2^{\operatorname{prec}(x)}}$ . If  $e^{-n}$  is computed with m bits, then the error on it is at most  $e^{-n}2^{1-m}$ . The error on r is then  $(n+1+2/n)2^{-\operatorname{prec}(x)}+\operatorname{ulp}(r)$ . Since  $x\geq \frac{2}{3}n$  for  $n\geq 2$ , and  $x2^{-\operatorname{prec}(x)}<\operatorname{ulp}(x)$ , this gives an error bounded by  $\operatorname{ulp}(r)+(n+1+2/n)\frac{3}{2n}\operatorname{ulp}(r)\leq 4\operatorname{ulp}(r)$  for  $n\geq 2$ — if  $\operatorname{prec}(x)=\operatorname{prec}(r)$ . Now since  $r\leq \frac{e^{-n}}{n}\leq \frac{1}{8}$ , that error is less than  $\operatorname{ulp}(1/2)$ .

FINAL COMPUTATION. We use the formula  $\gamma = S(n) - R(n) - \log n$  with n such that  $e^{-2n} \le \text{ulp}(1/2) = 2^{-\text{prec}}$ , i.e.  $n \ge \text{prec} \frac{\log 2}{2}$ :

$$s \leftarrow S'(n)$$
  
 $l \leftarrow \log(n)$   
 $r \leftarrow R'(n)$   
return  $(s - l) - r$ 

Since the final result is in  $[\frac{1}{2},1]$ , and  $R'(n) \leq \frac{e^{-n}}{n}$ , then S'(n) approximates  $\log n$ . If the target precision is m, and we use  $m + \lceil \log_2(\operatorname{prec}) \rceil$  bits to evaluate s and l, then the error on s-l will be at most  $\operatorname{3ulp}(1/2)$ , so the error on (s-l)-r is at most  $\operatorname{5ulp}(1/2)$ , and adding the  $3e^{-2n}$  truncation error, we get a bound of  $\operatorname{8ulp}(1/2)$ . [FIXME: check with new method to compute S]

5.2.1. A faster formula. Brent and McMillan give in [5] a faster algorithm (B2) using the modified Bessel functions, which was used by Gourdon and Demichel to compute 108,000,000 digits of  $\gamma$  in October 1999:

$$\gamma = \frac{S_0 - K_0}{I_0} - \log n,$$

where  $S_0 = \sum_{k=1}^{\infty} \frac{n^{2k}}{(k!)^2} H_k$ ,  $H_k = 1 + \frac{1}{2} + \cdots + \frac{1}{k}$  being the k-th harmonic number,  $K_0 = \sqrt{\frac{\pi}{4n}} e^{-2n} \sum_{k=0}^{\infty} (-1)^k \frac{[(2k)!]^2}{(k!)^3 (64n)^k}$ , and  $I_0 = \sum_{k=0}^{\infty} \frac{n^{2k}}{(k!)^2}$ . We have  $I_0 \ge \frac{e^{2n}}{\sqrt{4\pi n}}$  (see [5] page 306). From the remark following formula 9.7.2 of [1], the

We have  $I_0 \ge \frac{e^{2n}}{\sqrt{4\pi n}}$  (see [5] page 306). From the remark following formula 9.7.2 of [1], the remainder in the truncated expansion for  $K_0$  up to k does not exceed the (k+1)-th term, whence  $K_0 \le \sqrt{\frac{\pi}{4n}}e^{-2n}$  and  $\frac{K_0}{I_0} \le \pi e^{-4n}$  as in formula (5) of [5]. Let  $I_0' = \sum_{k=0}^{K-1} \frac{n^{2k}}{(k!)^2}$  with  $K = \lceil \beta n \rceil$ , and  $\beta$  is the root of  $\beta(\log \beta - 1) = 3$  ( $\beta \sim 4.971...$ ) then

$$|I_0 - I_0'| \le \frac{\beta}{2\pi(\beta^2 - 1)} \frac{e^{-6n}}{n}.$$

Let  $K'_0 = \sqrt{\frac{\pi}{4n}}e^{-2n}\sum_{k=0}^{4n-1}(-1)^k\frac{[(2k)!]^2}{(k!)^3(64n)^k}$ , then bounding by the next term:

$$|K_0 - K_0'| \le \frac{(8n+1)}{16\sqrt{2}n} \frac{e^{-6n}}{n} \le \frac{1}{2} \frac{e^{-6n}}{n}.$$

We get from this

$$\left| \frac{K_0}{I_0} - \frac{K_0'}{I_0'} \right| \le \frac{1}{2I_0} \frac{e^{-6n}}{n} \le \sqrt{\frac{\pi}{n}} e^{-8n}.$$

Let  $S_0' = \sum_{k=1}^{K-1} \frac{n^{2k}}{(k!)^2} H_k$ , then using  $\frac{H_{k+1}}{H_k} \leq \frac{k+1}{k}$  and the same bound K than for  $I_0'$   $(4n \leq K \leq 5n)$ , we get:

$$|S_0 - S_0'| \le \frac{\beta}{2\pi(\beta^2 - 1)} H_k \frac{e^{-6n}}{n}.$$

We deduce:

$$\left| \frac{S_0}{I_0} - \frac{S_0'}{I_0'} \right| \le e^{-8n} H_K \frac{\sqrt{4\pi n}}{\pi (\beta^2 - 1)} \frac{\beta}{n} \le e^{-8n}.$$

Hence we have

$$\left| \gamma - \left( \frac{S_0' - K_0'}{I_0'} - \log n \right) \right| \le (1 + \sqrt{\frac{\pi}{n}}) e^{-8n} \le 3e^{-8n}.$$

5.3. **The** log 2 **constant.** This constant is used in the exponential function, and in the base 2 exponential and logarithm.

We use the following formula (formula (30) from [9]):

$$\log 2 = \frac{3}{4} \sum_{n>0} (-1)^n \frac{n!^2}{2^n (2n+1)!}.$$

Let w be the working precision. We take  $N = \lfloor w/3 \rfloor + 1$ , and evaluate exactly using binary spitting:

$$\frac{T}{Q} = \frac{3}{4} \sum_{n>0}^{N-1} (-1)^n \frac{n!^2}{2^n (2n+1)!},$$

where T and Q are integers. Since the series has alternating signs with decreasing absolute values, the truncating error is bounded by the first neglected term, which is less than  $2^{-3N-1}$  for  $N \geq 2$ ; since  $N \geq (w+1)/3$ , this error is bounded by  $2^{-w-2}$ .

We then use the following algorithm:

 $t \leftarrow \circ(T)$  [rounded to nearest]

 $q \leftarrow \circ(Q)$  [rounded to nearest]

 $x \leftarrow \circ(t/q)$  [rounded to nearest]

Using Higham's notation, we write  $t=T(1+\theta_1),\ q=Q(1+\theta_2),\ x=t/q(1+\theta_3)$  with  $|\theta_i|\leq 2^{-w}$ . We thus have  $x=T/Q(1+\theta)^3$  with  $|\theta|\leq 2^{-w}$ . Since  $T/Q\leq 1$ , the total absolute error on x is thus bounded by  $3|\theta|+3\theta^2+|\theta|^3+2^{-w-2}<2^{-w+2}$  as long as  $w\geq 3$ .

5.4. Catalan's constant. Catalan's constant is defined by

$$G = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}.$$

We compute it using formula (31) of Victor Adamchik's document "33 representations for Catalan's constant" 4:

$$G = \frac{\pi}{8}\log(2+\sqrt{3}) + \frac{3}{8}\sum_{k=0}^{\infty} \frac{(k!)^2}{(2k)!(2k+1)^2}.$$

<sup>4</sup> http://www-2.cs.cmu.edu/~adamchik/articles/catalan/catalan.htm

Let  $f(k) = \frac{(k!)^2}{(2k)!(2k+1)^2}$ , and  $S(0,K) = \sum_{k=0}^{K-1} f(k)$ , and  $S = S(0,\infty)$ . We compute S(0,K) exactly by binary splitting. Since  $f(k)/f(k-1) = \frac{k(2k-1)}{2(2k+1)^2} \le 1/4$ , the truncation error on S is bounded by  $4/3f(K) \le 4/3 \cdot 4^{-K}$ . Since S is multiplied by 3/8, the corresponding contribution to the absolute error on G is  $2^{-2K-1}$ . As long as 2K+1 is greater or equal to the working precision w, this truncation error is less than one ulp of the final result.

```
K \leftarrow \lceil \frac{w-1}{2} \rceil
T/Q \leftarrow S(0, K) \text{ [exact, rational]}
T \leftarrow 3T \text{ [exact, integer]}
t \leftarrow \circ(T) \text{ [up]}
q \leftarrow \circ(Q) \text{ [down]}
s \leftarrow \circ(t/q) \text{ [nearest]}
x \leftarrow \circ(\sqrt{3}) \text{ [up]}
y \leftarrow \circ(2+x) \text{ [up]}
z \leftarrow \circ(\log y) \text{ [up]}
u \leftarrow \circ(\pi) \text{ [up]}
v \leftarrow \circ(uz) \text{ [nearest]}
q \leftarrow \circ(v+s) \text{ [nearest]}
Return \ g/8 \text{ [exact]}.
```

The error on t and q is less than one ulp; using the generic error on the division, since  $t \ge T$  and  $q \le Q$ , the error on s is at most 9/2 ulps.

The error on x is at most 1 ulp; since 1 < x < 2 — assuming  $w \ge 2$  —, ulp(x) = 1/2ulp(y), thus the error on y is at most 3/2ulp(y). The generic error on the logarithm (§2.9) gives an error bound of  $1 + \frac{3}{2} \cdot 2^{2-\exp(z)} = 4$  ulps for z (since  $3 \le y < 4$ , we have  $1 \le z < 2$ , so  $\exp(z) = 1$ ). The error on u is at most 1 ulp; thus using the generic error on the multiplication, since both u and z are upper approximations, the error on v is at most 11 ulps. Finally that on g is at most 11 + 9/2 = 31/2 ulps. Taking into account the truncation error, this gives 33/2 ulps.

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