NANZAN-TR-2008-01

Analysis of High-Precision Evaluation of Goursat's Infinite Integral

Yasuyo Hatano, Ichizo Ninomiya,
Hiroshi Sugiura, Takemitsu Hasegawa

November 2008

Technical Report of the Nanzan Academic Society
Mathematical Sciences and Information Engineering

Analysis of High-Precision Evaluation of Goursat's Infinite Integral

Yasuyo Hatano[*], Ichizo Ninomiya[†], Hiroshi Sugiura[‡], and Takemitsu Hasegawa[§]

November 5, 2008

Abstract

The infinite integral $\int_0^\infty x\,dx/(1+x^6\sin^2 x)$ is bounded but hard to evaulate because the integrand $f(x) = x/(1+x^6\sin^2 x)$ is a non-convergent and unbounded function, indeed $f(k\pi) = k\pi \to \infty$ $(k \to \infty)$. We show an efficient method to evaluate the above integral in high accurary and actually obtain an approximate value in up to 73 significant digits on an octuple precision system in C++.

1 Introduction

Many challenging problems in the numerical integration exist, say a challenging integral in the SIAM 100-Digit Challenge [2], which was also evaluated by Gautschi [6] and Slevinsky and Safouhi [14], and one due to Espelid [4]. The numerical evaluation of the infinite integral

$$I = \int_0^\infty f(x)dx, \quad f(x) = \frac{x}{1+x^6\sin^2 x} \tag{1}$$

might be also one of such hard problems to crack among other things. Toda of Chiba University challenged anyone to perform the numerical evaluation of I above at the conference held at the RIMS of Kyoto University in 1984. It is known, see Goursat [7, p.205], [8, p.182], Hardy [9, p.17], that although the function $f(x)$ (1) is non-convergent and unbounded when $x \to \infty$ since $f(k\pi) = k\pi$, as shown in Fig 1, the integral I approaches a limit. Indeed, we have $I = \sum_{n=0}^{\infty} I_n$,

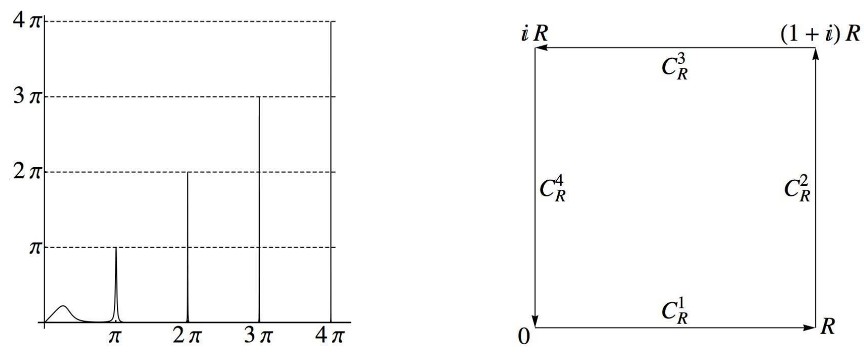

Figure 1: Integrand function $f(x) = x/(1+x^6\sin^2 x)$ (left) in (1) and the contour C_R (3)

[*]Chukyo University, Toyota, Aichi
[†]Professor Emeritus of Nagoya University, Nagoya
[‡]Nanzan University, Seto, Aichi
[§]University of Fukui, Fukui

where

$$\begin{aligned} I_n &:= \int_{n\pi}^{(n+1)\pi} \frac{x}{1+x^6\sin^2 x}dx < \int_0^{\pi} \frac{(n+1)\pi}{1+(n\pi)^6\sin^2 x}dx = 2\int_0^{\pi/2} \frac{(n+1)\pi}{1+(n\pi)^6\sin^2 x}dx \\ &= 2(n+1)\pi \frac{\tan^{-1}(\sqrt{1+(n\pi)^6}\tan x)}{\sqrt{1+(n\pi)^6}}\Big|_{x=0}^{x=\pi/2} = \frac{(n+1)\pi^2}{\sqrt{1+(n\pi)^6}} \sim \mathrm{O}(n^{-2}). \end{aligned} \tag{2}$$

It follows that the series $\sum_{n=0}^{\infty} I_n$ converges.

It appears that a simple method to evaluate I (1) is to compute the finite integrals I_n (2) by using some quadrature methods followed by applying some acceleration schemes such as the ρ-algorithm [3, p.102], [13, p.375] since the series $\sum_{n=0}^{\infty} I_n$ is a logarithmically convergent one. This scheme, however, proves to be unsuccessful, particularly to get the approximation value in high accuracy. In fact, Ninomiya [12] (1986) used the quadrature routine AQNN9 [11] and the ρ-algorithm in quadruple precision computation on the Fujitsu M-382 (about 26 significant digits) to obtain an approximate value to I (1) in about 20 significant digits.

The purpose of this paper is to propose a very efficient method to evaluate the integral I (1) in high accuracy without resort to acceleration methods. Present scheme is based on the contour integration to transform the original integral I (1) into another infinite integral much easier to approximate, see (5) and Fig 2 below. We evaluate the transformed integral by using the DE formula [15] and the summation of residuals of $f(z)$ at its poles on the complex plane $z = x + iy$. In computing the sum of the residuals, which is also of logarithmical convergence, we make use of the polygamma funcion [1, p.260] and its asymptotic expansion, see (31) and (38), instead of the ρ-algorithm. All computations are performed on an octuple precision system (more than 72 significant digits) in C++ due to Ninomiya.

This paper is organized as follows. In section 2 the integral I (1) is transformed into an infinite integral easy to approximate by using the contour integration, which requires the evaluation of residuals of $f(z)$ in (1) at poles in the first quadrant of the complex plane. Theorem 2.2 given in section 2 on the location of the poles is proven in section 3. In section 4 the poles of $f(z)$ and its residuals are evaluated. In section 5 we show the numerical result (41) in as much as 73 significant digits obtained by using an octuple precision system due to Ninomiya shown in Appendix A.

2 Contour integration and residuals

For a positive integer N let $R = (N + 1/2)\pi$ and C_R be a square contour on the complex plane $z = x + iy$ such that

$$\begin{aligned} C_R &= C_R^1 + C_R^2 + C_R^3 + C_R^4, \quad C_R^1 : z = t, \quad C_R^2 : z = R + it, \\ &\quad C_R^3 : z = -t + (1+i)R, \quad C_R^4 : z = (R-t)i, \quad 0 \le t \le R, \end{aligned} \tag{3}$$

as shown in Fig 1. Further let C be the contour around the first quadrant $x \ge 0, y \ge 0$ defined by

$$C = \lim_{N\to\infty} C_R. \tag{4}$$

Lemma 2.1 *Let C be the contour defined by (4) and let L be defined by*

$$L = \int_0^{\infty} \frac{y}{1+y^6\sinh^2 y}dy. \tag{5}$$

Then for $f(x)$ and I (1) we have

$$\oint_C f(z)dz = I + L. \tag{6}$$

proof. Since we have

$$\begin{aligned} \oint_{C_R} f(z)dz &= \int_{C_R^1} f(z)dz + \int_{C_R^2+C_R^3} f(z)dz + \int_{C_R^4} f(z)dz \\ &= \int_0^R f(t)dt + \int_{C_R^2+C_R^3} f(z)dz + i\int_R^0 f(it)dt, \end{aligned} \tag{7}$$

to establish the lemma it suffices to show that the second integral in the right hand side of (7) goes to zero when $R = (N + 1/2)\pi \to \infty$ because the first and last terms in the right hand side of (7) converge to I and L, respectively. The second integral is seen to converge to zero in the following way. Since

$$|\sin^2 z| = \sin^2 R + \sinh^2 t = 1 + \sinh^2 t \geq 1 \ (z \in C_R^2 : z = R + it),$$
$$|\sin^2 z| = \sin^2(R - t) + \sinh^2 R \geq \sinh^2 R \geq R^2 \geq 1 \ (z \in C_R^3 : z = R - t + iR),$$

we have

$$|f(z)| \leq \frac{\sqrt{2}R}{|z^6 \sin^2 z| - 1} \leq \frac{\sqrt{2}R}{R^6 - 1}, \quad (z \in C_R^2 + C_R^3).$$

From this relation it follows that

$$\Big| \int_{C_R^2 + C_R^3} f(z)dz \Big| \leq \int_{C_R^2 + C_R^3} |f(z)|\,|dz| \leq \frac{2\sqrt{2}R^2}{R^6 - 1} \to 0, \quad (N \to \infty). \qquad \square$$

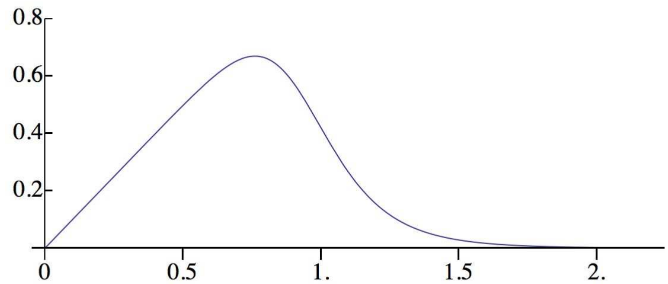

Figure 2: Function $x/(1 + x^6 \sinh^2 x)$ for the integral L (5)

Now we compute the residuals at the poles of $f(z)$ to evaluate $\oint_C f(z)dz$ in (6).

Theorem 2.2 *Let E be a region consisting of disks E_n arranged along the real line of the complex plane, defined by*

$$\begin{aligned} E \quad &= \quad \bigcup_{n=-\infty}^{\infty} E_n, \quad E_n = \{|z - n\pi| < a_{|n|}\} \ (n = 0, \pm 1, \pm 2, \cdots), \\ & \quad\ \ a_0 = 1.05, \quad a_n = (3n)^{-3} \ (n \geq 1). \end{aligned} \tag{8}$$

Let $g(z) = 1 + z^6 \sin^2 z$. Then $g(z)$ has simple zeros only in E and no multiple zeros, in particular eight in E_0 and two in each E_n $(n \neq 0)$.

The proof of Theorem 2.2 is given in section 3 below. Since if ζ is a zero of $g(z) = 1 + z^6 \sin^2 z$, then $-\zeta$ and $\pm\overline{\zeta}$ are also zeros of $g(z)$, we have the following corollary.

Corollary 2.3 *In the first quadrant of the complex plane $z = x + iy$, namely $x \geq 0$, $y \geq 0$, the function $f(z) = z/(1 + z^6 \sin^2 z)$ has two simple poles z_{-1} and z_0 in E_0 and only z_n in each E_n $(n \geq 1)$.*

From (6) and Corollary 2.3 we have

$$I = \oint_C f(z)dz - L = \Re 2\pi i \sum_{n=-1}^{\infty} \lambda_n - L = -2\pi \sum_{n=-1}^{\infty} \Im \lambda_n - L, \tag{9}$$

where the residues λ_n of $f(z)$ at the poles $z = z_n$ $(n \geq -1)$ are given by

$$\lambda_n = \lim_{z \to z_n} \frac{(z - z_n)\, z}{1 + z^6 \sin^2 z} = \lim_{z \to z_n} \frac{2z - z_n}{2z^6 \sin z \cos z + 6z^5 \sin^2 z} = \frac{-z_n}{2 \cot z_n + 6z_n^{-1}}, \tag{10}$$

since z_n $(n \geq -1)$ satisfy $1 + z_n^6 \sin^2 z_n = 0$.

3 Proof of Theorem 2.2

We start by proving that $g(z)$ has no zeros in E^c, the compliment of E. Since $g(z)$ is an even function it suffices to show that $h(z) := |z^3 \sin z| > 1$ on $E^c \cap \{z | \Re z \geq -a_0\}$. Let ∂E_n be the boundary of E_n and define the line segments I_n on the real line by

$$I_n = [n\pi + a_n, (n+1)\pi - a_{n+1}], \quad n \geq 0.$$

Further let $J = \cup_{n=0}^{\infty} (\partial E_n \cup I_n)$ and $z = x + iy$. Then it suffices to show that $h(z) > 1$ on J since $h(z)$, that is written as follows

$$h(z) = (x^2 + y^2)^{3/2} (\sin^2 x + \sinh^2 y)^{1/2},$$

is a monotone increasing function with respect to $|y|$.

Now we consider an union $\cup_{n=0}^{\infty} A_n$ of annular regions A_n including J, where

$$A_n = \{a_n \leq |z - n\pi| \leq b_n\}, \quad b_n = \pi - a_{|n-1|} \ (n \geq 0), \tag{11}$$

as shown in Fig 3. Then we show that $h(z) > 1$ in $\cup_{n=0}^{\infty} A_n$, namely $h(n\pi + re^{i\theta}) > 1$, where

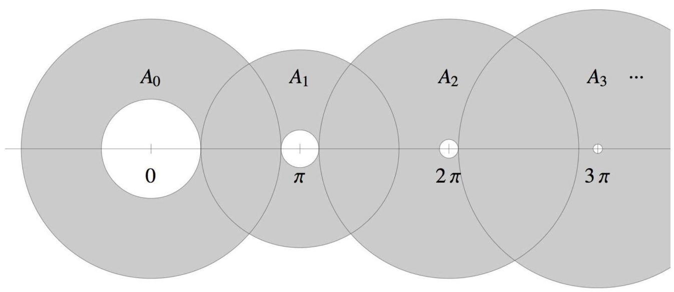

Figure 3: Union of annular regions

$a_n \leq r \leq b_n < \pi$ $(n \geq 0)$ and $0 \leq \theta \leq 2\pi$. Let $z = n\pi + re^{i\theta}$ $(0 \leq r \leq \pi, 0 \leq \theta \leq 2\pi)$, then

$$h(z) = h(n\pi + re^{i\theta}) = |n\pi + re^{i\theta}|^3 \, |\sin(re^{i\theta})| \geq |n\pi - r|^3 \sin r, \tag{12}$$

since noting that

$$\sin x \geq x (\sin r)/r \ (0 \leq x \leq r < \pi), \quad \sinh x \geq x \ (x \geq 0), \quad r \geq \sin r \ (r \geq 0),$$

we have

$$\begin{aligned} |\sin(re^{i\theta})|^2 &= \sin^2(r\cos\theta) + \sinh^2(r\sin\theta) \geq \{r\cos\theta\,(\sin r)/r\}^2 + r^2 \sin^2\theta \\ &= \sin^2 r + (r^2 - \sin^2 r)\sin^2\theta \geq \sin^2 r. \end{aligned} \tag{13}$$

Define $u(r)$ and $v(r)$ by, respectively

$$u(r) = \sin r, \quad v(r) = 1/|n\pi - r|^3, \quad 0 \leq r \leq \pi, \tag{14}$$

then from (12) we have $h(z) \geq u(r)/v(r)$. Since $v(r)$ and $u(r)$ are convex and concave functions on $0 \leq r \leq \pi$, respectively and further $u(0) = 0 < v(0)$, $u(\pi) = 0 < v(\pi)$ and $v(\pi/2) < u(\pi/2) = 1$ there exist c_n and d_n such that

$$u(c_n) = v(c_n), \quad u(d_n) = v(d_n), \quad u(r) > v(r), \ (0 < c_n < r < d_n < \pi).$$

It immediately follows that $h(z) \geq u(r)/v(r) > 1$ $(c_n < r < d_n)$. It remains to show that $c_n \leq a_n$ and $b_n \leq d_n$. To this end it suffices to show that $u(a_n)/v(a_n) > 1$ and $u(b_n)/v(b_n) > 1$.

Recall that $a_0 = 1.05$ and $a_n = (3n)^{-3}$ $(n \geq 1)$. Then it is easy to see that $u(a_n)/v(a_n) > 1$ since $u(a_0)/v(a_0) = (1.05)^3 \sin(1.05) = 1.004\cdots > 1$ and by using the relation that $\sin x \geq 3x/\pi$ $(0 \leq x \leq \pi/6)$ we have for $n \geq 1$

$$\begin{aligned}\frac{u(a_n)}{v(a_n)} &= \{n\pi - (3n)^{-3}\}^3 \sin\{(3n)^{-3}\} \geq \{n\pi - (3n)^{-3}\}^3 \frac{3}{\pi}(3n)^{-3} \\ &\geq \frac{\pi^2}{9}\Big\{1 - \frac{1}{n\pi(3n)^3}\Big\}^3 > 1.058\cdots > 1. \qquad (15)\end{aligned}$$

On the other hand, since from (11) and (14) we have

$$\frac{u(b_n)}{v(b_n)} = |(n-1)\pi + a_{|n-1|}|^3 \sin(a_{|n-1|}),$$

it follows in the way similar to (15) that $u(b_n)/v(b_n) > 1$ for $n \geq 2$ and $n = 0$, while for $n = 1$ we have $u(b_1)/v(b_1) = u(a_0)/v(a_0)$, which is greater than unity as shown above.

Since $|z^6 \sin^2 z| > 1$ on ∂E_n $(n \geq 0)$ as shown above and $z^6 \sin^2 z$ has 8 zeros in E_0 and 2 in each E_n $(n \geq 1)$, we can use Rouché's theorem [10, p.280] to show that $g(z) = 1 + z^6 \sin^2 z$ has 8 zeros in E_0 and 2 in each E_n $(n \geq 1)$.

Finally we prove that all zeros of $g(z)$ are simple zeros as follows; the assumption that $g(z)$ has at least a double zero at $z = \zeta$ in E_n leads to the contradiction. The assumption immediately gives

$$\begin{aligned} g(\zeta) &= 1 + \zeta^6 \sin^2 \zeta = 0, \qquad (16)\\ g'(\zeta) &= 6\zeta^5 \sin^2 \zeta + 2\zeta^6 \sin\zeta \cos\zeta = 0. \qquad (17)\end{aligned}$$

Since $\zeta \neq 0$ and $\sin\zeta \neq 0$, from (16) and (17) we have $\sin^2 \zeta = -\zeta^{-6}$ and $\cos^2 \zeta = (-3\zeta^{-1} \sin\zeta)^2 = -9\zeta^{-8}$, which give the relation

$$\zeta^8 + \zeta^2 = -9. \qquad (18)$$

If $\zeta \in E_0$, then (18) is invalid because $|\zeta|^8 + |\zeta|^2 < (1.05)^8 + (1.05)^2 < 9$. If ζ is in E_n $(n \geq 1)$, then $\overline{\zeta}$ is another zero in E_n and $\overline{\zeta} \neq \zeta$ because $g(z)$ has no real zeros. Thus we have four zeros (counting the multiplicity) instead of two. □

4 Evaluation of the poles and the residuals

Now we start by determining the location of the poles z_n $(n \geq -1)$ in the first quadrant. Two poles z_{-1} and z_0 in E_0 are zeros of $z^3 \sin z + i$ and $z^3 \sin z - i$, respectively and are given by using the Newton method as follows

$$z_{-1} = 0.34901\cdots + i\,0.90654\cdots, \quad z_0 = 0.936399\cdots + i\,0.42672\cdots.$$

On the other hand, z_n in E_n $(n \geq 1)$ are zeros of $z^3 \sin z - (-1)^n i$. To verify this letting $w = (n\pi)^{-1}$ and $z_n = n\pi + \rho = w^{-1} + \rho$ we find the value of $\rho(w)$ satisfying $(w^{-1} + \rho)^3 \sin\rho = i$.

Lemma 4.1 *For a complex w such that $|w| \leq 5/9$ there exists only one solution $\rho(w)$ of*

$$\sin\rho = iw^3/(1 + w\rho)^3, \qquad (19)$$

in $|\rho| < 1/3$. Further $\rho(w)$ is an odd analytic function on $|w| \leq 5/9$ and has the Maclaurin expansion,

$$\rho(w) = \sum_{k=0}^{\infty} a_k\, w^{2k+1} = iw^3 + 3w^7 - \frac{i}{6}w^9 - 15iw^{11} - 2w^{13} + \cdots, \qquad (20)$$

with $|a_k| \leq (9/5)^{2k+1}/3$.

Proof. It is trivial that $\rho(w)$ is an odd function because (19) holds also for $-w$ and $-\rho$. We proceed to show that (19) has only one solution in $|\rho| \leq 1/3$ by using Rouché's theorem. Since $\sin\rho$ has only one zero in $|\rho| < 1/3$, it is required to show that $|\sin\rho| > |iw^3/(1+w\rho)^3|$ on $|\rho| = 1/3$. Since from (13) and the relation $|w| \leq 5/9$ we can verifty that $|\sin\rho| \geq \sin|\rho|$ and $\sin(1/3) > |w|^3/(1-|w|/3)^3$, it follows that for $|w| \leq 5/9$ and $|\rho| = 1/3$

$$|\sin\rho| \geq \sin|\rho| = \sin(1/3) > \frac{|w|^3}{(1-|w|/3)^3} = \frac{|w|^3}{(1-|w\rho|)^3} \geq \Big|\frac{iw^3}{(1+w\rho)^3}\Big|.$$

Next we show that $\rho(w)$ is analytic in the disk $|w| \leq 5/9$. To this end it suffices to show that $|\rho'(w)| < \infty$ when $|\rho(w)| < 1/3$ and $|w| \leq 5/9$. Since differentiating the both sides of $(1+w\rho)^3 \sin\rho = iw^3$, which is derived from (19), with respect to w gives

$$3(w\rho' + \rho)(1+w\rho)^2 \sin\rho + \rho'(1+w\rho)^3 \cos\rho = 3iw^2,$$

it follows that

$$\rho'(w) = \frac{3iw^2 - 3\rho(1+w\rho)^2 \sin\rho}{(1+w\rho)^3\cos\rho + 3w(1+w\rho)^2 \sin\rho}.$$

To show that $|\rho'(w)| < \infty$ we verify that the denominator of the right hand side above has no zeros for $|w| \leq 5/9$. This is seen as follows. By using (19) we have

$$\begin{aligned}
&|(1+w\rho)^3\cos\rho + 3w(1+w\rho)^2\sin\rho| \\
&= \Big|(1+w\rho)^3\sqrt{1+w^6/(1+w\rho)^6} + 3w(1+w\rho)^2\frac{iw^3}{(1+w\rho)^3}\Big| \\
&\geq (1-|w\rho|)^3\sqrt{1-|w|^6/(1-|w\rho|)^6} - 3|w|^4/(1-|w\rho|) \\
&\geq (1-5/(9\times 3))^3\sqrt{1-(5/9)^6/(1-5/(9\times 3))^6} - 3(5/9)^4/(1-5/(9\times 3)) \\
&= 0.16\cdots > 0.
\end{aligned}$$

Since as shown above $\rho(w)$ is verified to be an analytic odd function in $|w| \leq 5/9$ on the complex plane w, we have the Taylor expansion of $\rho(w)$ in the form of (20), where by recalling that $|\rho(w)| < 1/3$ we have

$$|a_k| = \Big|\frac{\rho^{(2k+1)}(0)}{(2k+1)!}\Big| \leq \frac{1}{2\pi}\oint_{|w|=5/9}\Big|\frac{\rho(w)}{w^{2k+2}}\Big||dw| \leq \frac{1}{3}\Big(\frac{5}{9}\Big)^{-2k-1}.$$

The exact values of the coefficients a_k in (19) are obtained as follows. We note that $\rho = O(w)$ since $\rho = 0$ in (19) when $w = 0$. Expanding both sides of (19) yields

$$\sum_{k=0}^{\infty}\frac{(-1)^k\rho^{2k+1}}{(2k+1)!} = iw^3\sum_{k=0}^{\infty}\frac{(1+k)(2+k)}{2}(-w\rho)^k. \tag{21}$$

By substituting the expansion of $\rho(w)$ in the form of $\sum_{k=0}^{\infty} a_k w^{2k+1}$ as shown in (20) into both sides of (21) and comparing the coefficients of w^{2k+1} we have the rightmost hand side of (20). This manipulation of the equations was carried out by using Mathematica. $\square$

Using $w = (n\pi)^{-1}$ in Lemma 4.1 gives the following Corollary.

Corollary 4.2 *Let $f(z)$ be a function defined by (1) and E_n be regions defined by (8). Then the poles $z_n \in E_n$ in the first quadrant of $f(z)$ are given by*

$$\begin{aligned}
z_n &= n\pi + \rho\Big(\frac{1}{n\pi}\Big) = n\pi + \sum_{k=0}^{\infty}\frac{a_k}{(n\pi)^{2k+1}} \\
&= n\pi + \frac{i}{(n\pi)^3} + \frac{3}{(n\pi)^7} - \frac{i}{6(n\pi)^9} - \frac{15i}{(n\pi)^{11}} - \frac{2}{(n\pi)^{13}} + \cdots, \quad n \geq 1.
\end{aligned} \tag{22}$$

From (22) we can verify that $z_n \in E_n$ in the first quadrant, namely $|z_n - n\pi| \le 1/(3n)^3$ $(n \ge 1)$ and $\Im z_n > 0$ as follows. By noting that

$$\Big|\sum_{k=4}^{\infty} \frac{a_k}{(n\pi)^{2k+1}}\Big| \le \frac{1}{3}\sum_{k=4}^{\infty}\Big(\frac{9}{5n\pi}\Big)^{2k+1} = \frac{1}{3}\Big(\frac{9}{5n\pi}\Big)^{9}\frac{1}{1-\{9/(5n\pi)\}^2} < \frac{0.11}{(n\pi)^3},$$

it follows that

$$|z_n - n\pi| \le \frac{1}{(n\pi)^3} + \frac{3}{(n\pi)^7} + \frac{0.11}{(n\pi)^3} < \frac{1}{27.17n^3} < \frac{1}{(3n)^3},$$

and

$$\Im z_n > \frac{1}{(n\pi)^3} - \frac{0.11}{(n\pi)^3} > 0.$$

Lemma 4.3 *Let $\rho(w)$ be a solution of (19). Let $\lambda(w)$ be defined by*

$$\lambda(w) = \frac{-\{w^{-1}+\rho(w)\}}{2\cot\rho(w) + 6\{w^{-1}+\rho(w)\}^{-1}}. \tag{23}$$

Then $\lambda(w)$ is an analytic even function with $|\lambda(w)| < 1/3$ when $|w| \le 5/9$ and is expanded as follows

$$\lambda(w) = \sum_{k=0}^{\infty} b_k w^{2k} = -\frac{i}{2}w^2 - \frac{5}{2}w^6 + \frac{i}{4}w^8 + 18iw^{10} + \frac{11}{3}w^{12} + \cdots, \tag{24}$$

where $|b_k| \le 5(9/5)^{2k}/3$.

Proof. Since $\rho(-w) = -\rho(w)$ as shown in Lemma 4.1 we can verify that $\lambda(w)$ (23) is an even function, $\lambda(-w) = \lambda(w)$. We proceed to show that $\lambda(w)$ is analytic in $|w| \le 5/9$. To this end we verify that $\lambda(w)$ has no poles in $|w| \le 5/9$. From (23) and (19) it follows that

$$\lambda(w) = \frac{-(1+w\rho)^2 w^{-1}\sin\rho}{2(1+w\rho)\cos\rho + 6w\sin\rho} = \frac{-i(1+w\rho)^2 w^2}{2(1+w\rho)^4\sqrt{1+w^6/(1+w\rho)^6} + 6iw^4}. \tag{25}$$

We see that the denominator of the rightmost hand side of (25) has no zeros in $|w| \le 5/9$ since noting that $|\rho| < 1/3$ and $|w\rho| \le 5/27$ we have

$$\begin{aligned} &|2(1+w\rho)^4\sqrt{1+w^6/(1+w\rho)^6} + 6iw^4| \\ &\quad \ge 2(1-5/27)^4\sqrt{1-(5/9)^6/(1-5/27)^6} - 6(5/9)^4 = 0.2645728\cdots > 0. \end{aligned} \tag{26}$$

Since from (25) and (26) we see that

$$|\lambda(w)| \le \frac{(1+5/27)^2(5/9)^2}{0.2645728\cdots} = 1.6386\cdots < \frac{5}{3},$$

similarly to the derivation of the bound of $|a_k|$ in Lemma 4.1 we can verify that $|b_k| \le 5(9/5)^{2k}/3$. The exact values of the coefficients b_k in (24) are obtained by using $\rho(w)$ (20) in (25) followed by the expansion in terms of w. This manipulation of the equation was also carried out by using Mathematica. □

From Lemma 4.3 we have the following corollary.

Corollary 4.4 *Let λ_n be the residue of $f(z) = z/(1+z^6\sin^2 z)$ at the pole $z_n \in E_n$. Then we have for $n \ge 1$*

$$\lambda_n = \sum_{k=0}^{\infty}\frac{b_k}{(n\pi)^{2k}} = -\frac{i}{2(n\pi)^2} - \frac{5}{2(n\pi)^6} + \frac{i}{4(n\pi)^8} + \frac{18i}{(n\pi)^{10}} + \frac{11}{3(n\pi)^{12}} + \cdots. \tag{27}$$

Using above λ_n in (9) we have

$$I = \int_0^\infty \frac{x}{1+x^6\sin^2 x}dx = \sum_{n=-1}^{\infty} \mu_n - \int_0^\infty \frac{x}{1+x^6\sinh^2 x}dx, \tag{28}$$

where $\mu_n = \Re(2\pi i \lambda_n) = -2\pi \Im \lambda_n$, particularly

$$\mu_n = \sum_{k=1}^{\infty} \frac{c_k}{(n\pi)^{2k}} = \frac{\pi}{(n\pi)^2} - \frac{\pi}{2(n\pi)^8} - \frac{36\pi}{(n\pi)^{10}} + \frac{3\pi}{8(n\pi)^{14}} + \cdots, \quad n \geq 1, \tag{29}$$

and $|c_k| \leq 10\pi(9/5)^{2k}/3$.

Lemma 4.5 *Let μ_n $(n \geq 1)$ be given by (29). For positive integers m and N let $\widetilde{S}_N$, $\widetilde{S}_N^{(m)}$ and $\mu_n^{(m)}$ $(n \geq 1)$ be defined by*

$$\widetilde{S}_N = \sum_{n=N+1}^{\infty} \mu_n, \quad \widetilde{S}_N^{(m)} = \sum_{n=N+1}^{\infty} \mu_n^{(m)}, \quad \mu_n^{(m)} = \sum_{k=1}^{m} \frac{c_k}{(n\pi)^{2k}}, \tag{30}$$

respectively, where c_k is given by (29). Then we have

$$\widetilde{S}_N^{(m)} = \sum_{k=1}^{m} \frac{c_k \psi^{(2k-1)}(N+1)}{(2k-1)!\pi^{2k}}, \tag{31}$$

where $\psi^{(k)}(z)$ is the polygamma function [1, p.260]. Further we have

$$|\widetilde{S}_N^{(m)} - \widetilde{S}_N| \leq \frac{4N\pi}{2m+1}\Big(\frac{9}{5N\pi}\Big)^{2m+2}. \tag{32}$$

Proof. Since the polygamma function $\psi^{(k)}(z)$ is defined by

$$\psi^{(k)}(z) = (-1)^{k+1}k! \sum_{n=0}^{\infty} \frac{1}{(z+n)^{k+1}}, \quad z \neq 0, -1, -2, \ldots, \tag{33}$$

see [1, p.260, 6.4.10], from (30) it follows that

$$\widetilde{S}_N^{(m)} = \sum_{k=1}^{m} \frac{c_k}{\pi^{2k}} \sum_{n=N+1}^{\infty} \frac{1}{n^{2k}} = \sum_{k=1}^{m} \frac{c_k}{\pi^{2k}} \sum_{n=0}^{\infty} \frac{1}{(N+n+1)^{2k}} = \sum_{k=1}^{m} \frac{c_k \psi^{(2k-1)}(N+1)}{(2k-1)!\,\pi^{2k}}.$$

Since from (29) and (30) we have for $n \geq 2$

$$\begin{aligned} |\mu_n^{(m)} - \mu_n| &\leq \sum_{k=m+1}^{\infty} \frac{|c_k|}{(n\pi)^{2k}} \leq \sum_{k=m+1}^{\infty} \frac{10\pi}{3}\Big(\frac{9}{5}\Big)^{2k} \frac{1}{(n\pi)^{2k}} \\ &= \frac{10\pi}{3}\Big(\frac{9}{5n\pi}\Big)^{2m+2} \frac{1}{1-\{9/(5n\pi)\}^2} < 4\pi\Big(\frac{9}{5n\pi}\Big)^{2m+2}, \end{aligned}$$

it follows that

$$\begin{aligned} |\widetilde{S}_N^{(m)} - \widetilde{S}_N| &\leq \sum_{n=N+1}^{\infty} |\mu_n^{(m)} - \mu_n| < 4\pi\Big(\frac{9}{5\pi}\Big)^{2m+2} \sum_{n=N+1}^{\infty} \frac{1}{n^{2m+2}} \\ &< 4\pi\Big(\frac{9}{5\pi}\Big)^{2m+2} \int_N^\infty x^{-2m-2}dx = 4\pi\Big(\frac{9}{5\pi}\Big)^{2m+2} \frac{N^{-2m-1}}{2m+1}, \end{aligned}$$

from which we can verify (32). $\square$

Corollary 4.6 *For $\widetilde{S}_N$ and $\widetilde{S}_N^{(m)}$ (31) let S and $S_N^{(m)}$ be defined by*

$$S = \sum_{n=-1}^{\infty} \mu_n = \sum_{n=-1}^{N} \mu_n + \widetilde{S}_N, \quad S_N^{(m)} = \sum_{n=-1}^{N} \mu_n + \widetilde{S}_N^{(m)}, \tag{34}$$

respectively. Then the error of the approximation $S_N^{(m)}$ to S is given by

$$|S_N^{(m)} - S| = |\widetilde{S}_N^{(m)} - \widetilde{S}_N| \le \frac{4N\pi}{2m+1}\Big(\frac{9}{5N\pi}\Big)^{2m+2} := E_N^{(m)}. \tag{35}$$

5 Computed results in octuple precision

All computations in this section were carried out on the IBM ThinkCentre S50 ultra small (Intel Pentium 4 3.20GHz) with Microsoft Windows XP (Professional version 2002), in more than 72 significant digits by using an octuple precision system in Borland C++ 5.0, due to Ninomiya described in Appendix A. Furthermore, all computed results are compared in accuracy with ones in about 100 significant digits obtained by using Mathematica (ver. 6.0.1.0) on the iMac (2.16GHz, Inter Core 2 Duo) with Mac OS X (ver. 10.5.4).

5.1 Computation of the transformed integral

The numerical evaluation of the transformed integral L (5) is performed by using the DE formula due to Takahasi and Mori [15], which is known to be an efficient quadrature method for infinite integrals or integrals of singular functions. See also Evans [5, p.182]. Among the DE formulas we choose the one based on the change of variables $x = \varphi(t) = \exp(\alpha\, t - \beta e^{-t})$ for the integral $\int_0^\infty g(x)dx = \int_{-\infty}^\infty g(\varphi(t))\varphi'(t)dt \approx \int_a^b g(\varphi(t))\varphi'(t)dt$ since $g(x) = x/(1 + x^6 \sinh^2 x)$ behaves like e^{-x} $(x \to \infty)$. In our case we determine the values of a and b so that $|g(\varphi(t))\varphi'(t)| \le 10^{-72}$ at $t = a$ and b. In the original DE formula [15] $\alpha = \beta = 1$. Comprehensive numerical experiments, however, reveal that the choice of $\alpha = 0.22$, $\beta = 0.017$, $a = -8.5$ and $b = 19.7$ could approximate the transformed integral with nearly minimal number of function evaluations. Figure 4 depicts $g(\varphi(t))\varphi'(t)$. An approximation to L shown in (36) with correct digits in bold face is obtained

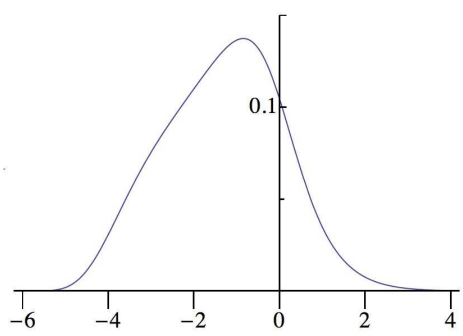

Figure 4: The function $g(\varphi(t))\varphi'(t)$ transformed by the DE formula, where $\varphi(t) = \exp(0.22\,t - 0.017\,e^{-t})$

with 480 function evaluations; the computing time is 0.640 seconds,

$$\begin{aligned} L &= \int_0^\infty \frac{x}{1 + x^6 \sinh^2 x} dx \\ &\approx \mathbf{5.}\ \ \mathbf{03686\ 66423\ 91385\ 10865\ 43394\ 94593\ 84622\ 05051} \\ &\qquad \mathbf{14197\ 98536\ 76323\ 79182\ 23941\ 37520}\ \mathit{5248} \times 10^{-1}. \end{aligned} \tag{36}$$

5.2 Computation of the residuals and the integral

We start by obtaining within the accuracy 10^{-72} the approximation $S_N^{(m)}$ to $S = \sum_{n=-1}^{\infty} \mu_n = -2\pi\Im\sum_{n=-1}^{\infty} \lambda_n$, (34). To this end we seek a set of N and m such that the error estimation $E_N^{(m)}$ in (35) is less than 10^{-72}. The choice of $N = 90$ and $m = 16$ might satisfy the condition above because $E_{90}^{(16)} = 360\pi\{9/(450\pi)\}^{34}/33 = 7.359\cdots\times 10^{-74}$. From (31) and (34) it follows that

$$S_{90}^{(16)} = \sum_{n=-1}^{90} \mu_n + \widetilde{S}_{90}^{(16)} = \sum_{n=-1}^{90} \mu_n + \sum_{k=1}^{16} \frac{c_k \psi^{(2k-1)}(91)}{(2k-1)!\,\pi^{2k}}, \tag{37}$$

where the polygamma function $\psi^{(k)}(n)$ is approximated by the truncation of the asymptotic expansion [1, p.260, 6.4.11] as follows

$$\psi^{(k)}(n) \approx (-1)^{k-1}\Big\{\frac{(k-1)!}{n^k} + \frac{k!}{2n^{k+1}} + \sum_{j=1}^{M} \frac{B_{2j}\,(2j+k-1)!}{(2j)!\,n^{2j+k}}\Big\} \tag{38}$$

with $n = N + 1 = 91$. Here B_j is the Bernoulli number. We choose $M = 38$ so that the relative error of the truncated expansion of $\psi^{(31)}(91)$, which converges at the slowest rate among $\psi^{(k)}(91)$ $(1 \le k \le 31)$, is within 10^{-73}. The coefficients c_k $(1 \le k \le 16)$ in (37) are given as follows

$$\begin{aligned}
c_1 &= \pi, \quad c_2 = c_3 = c_6 = 0, \quad c_4 = -\frac{\pi}{2}, \quad c_5 = -36\pi, \quad c_7 = \frac{3\pi}{8}, \\
c_8 &= \frac{175\pi}{2}, \quad c_9 = 2380\pi, \quad c_{10} = -\frac{5\pi}{16}, \quad c_{11} = -\frac{1813\pi}{12}, \quad c_{12} = -\frac{61985\pi}{6}, \\
c_{13} &= -\frac{22668765\pi}{128}, \quad c_{14} = \frac{125931\pi}{560}, \quad c_{15} = \frac{1116297\pi}{40}, \quad c_{16} = \frac{282731841\pi}{256}.
\end{aligned}$$

To compute $\mu_n = -2\pi\Im\lambda_n$ $(-1 \le n \le 90)$ in (37) we use the relation (10) for λ_n $(n = -1, 0)$ and $\lambda_n = -z_n/(2\cot\rho_n + 6z_n^{-1})$ for $z_n = n\pi + \rho_n$ $(n \ge 1)$. The poles z_n $(-1 \le n \le 90)$ are computed by the Newton method as follows. As shown in section 4 the first pole z_{-1} satisfies $z^3 \sin z + i = 0$. We choose the starting value $z_{-1}^{(0)} = e^{3\pi i/8}$ to get the approximate value $z_{-1}^{(6)}$ in 72 significant digit with 6 Newton iterations. On the other hand, since z_0 satisfies $z^6 \sin z - i = 0$, we get an approximation $z_0^{(6)}$ with 6 Newton iterations from the starting value $z_0^{(0)} = e^{\pi i/8}$. Further $z_n = n\pi + \rho_n$ $(1 \le n \le 90)$ satisfy $(n\pi + \rho)^3 \sin\rho - i = 0$. We choose the first five terms in the rightmost hand side of (22) as the starting values $z_n^{(0)}$, particularly

$$z_n^{(0)} = n\pi + \frac{i}{(n\pi)^3} + \frac{3}{(n\pi)^7} - \frac{i}{6(n\pi)^9} - \frac{15i}{(n\pi)^{11}},$$

to get approximations $z_n^{(\nu)}$ with ν Newton iterations, where $\nu = 4$ for $n = 1$ and $\nu = 2$ or 3 for $n \ge 2$.

The computed results of μ_n are shown in Table 1. The first and second sums in the rightmost hand side of (37) are obtained, respectively, as follows,

$$\begin{aligned}
\sum_{n=-1}^{90} \mu_n \approx \mathbf{1.}\ &\mathbf{66982\ 20179\ 37495\ 59342\ 43810\ 62820\ 58234\ 02421} \\
&\mathbf{49355\ 72174\ 81564\ 19168\ 12665\ 26574\ 95}\mathit{92},
\end{aligned} \tag{39}$$

$$\begin{aligned}
\widetilde{S}_{90}^{(16)} \approx \mathbf{3.}\ &\mathbf{51720\ 05261\ 29395\ 16697\ 54683\ 00000\ 04139\ 68434} \\
&\mathbf{80739\ 50322\ 48919\ 21611\ 20210\ 12285\ 8}\mathit{474} \times 10^{-3}.
\end{aligned} \tag{40}$$

n	μ_n
-1	4.45332 31717 50168 32554 91301 21231 12069 88558 06448 88090 33102 14635 45431 1348e-01
0	7.05771 74510 25032 78695 97574 99471 28453 17041 52586 66925 91819 99928 68958 7567e-01
1	3.16948 14281 17370 83919 71032 11864 78065 70501 79218 91903 94807 27589 09124 9931e-01
2	7.95756 45585 35577 97204 66587 47945 36103 96705 56364 43457 04952 99555 34631 0375e-02
3	3.53677 19447 44917 50202 92186 89287 11325 04365 18317 46231 12809 86732 87609 3055e-02
$\vdots$	$\vdots$
10	3.18309 88600 61669 82323 55258 19746 20809 93776 54660 45089 96567 01135 58007 3520e-03
11	2.63066 02155 76114 51927 82135 31277 05151 50863 00011 40185 41919 81782 87333 3180e-03
$\vdots$	$\vdots$
20	7.95774 71545 28920 67422 22610 74735 65347 35026 63029 18370 26090 93939 83161 6402e-04
21	7.21791 12512 88628 77541 73784 85305 93011 86603 03873 80612 89998 45263 43714 7420e-04
$\vdots$	$\vdots$
30	3.53677 65131 50686 03625 66840 70888 25775 21297 51364 52321 03211 25160 72747 5049e-04
31	3.31227 76918 16885 79262 13823 19378 08964 92238 79440 19633 02643 61049 49067 3903e-04
$\vdots$	$\vdots$
40	1.98943 67886 48437 94094 16605 62387 90476 96723 13020 89368 35701 23377 41814 9239e-04
41	1.89357 45757 51074 77150 88874 39357 14628 41047 90703 87687 28575 68407 05642 7354e-04
$\vdots$	$\vdots$
89	4.01855 68259 53671 73496 03578 33871 64640 73912 82900 25256 78499 85719 90648 8962e-05
90	3.92975 16812 81362 46606 94996 63700 92952 80420 32711 66147 64618 59260 36240 9424e-05

Table 1: Values of μ_n

From (28), (34), (36), (37), (39) and (40), we have an approximation to I (1) in 73 significant digits as follows

$$\begin{aligned} I = \int_0^\infty \frac{x}{1+x^6 \sin^2 x} dx &\approx \sum_{n=-1}^{90} \mu_n + \widetilde{S}_{90}^{(16)} - L \\ &\approx \mathbf{1.}\ \ \mathbf{16965\ 25542\ 24486\ 47772\ 59225\ 81661\ 19775\ 95884} \\ &\quad\ \ \mathbf{81416\ 66271\ 46180\ 73171\ 51391\ 33835\ 19}\mathit{30}. \end{aligned} \tag{41}$$

The total computing time required to obtain the approximation in (41) is 1.062 seconds.

Remark. We note that the use of $\widetilde{S}_N^{(m)}$, namely the polygamma function, instead of the acceleration method, plays an important role to approximate the sum S (34) in 73 significant digits. Indeed, when we apply the ρ-algorithm to the sequence of the finite sums $\sum_{n=M}^{N} \mu_n$ ($M \leq N \leq 120$), where M is a fixed integer in $[-1, 10]$, we obtain the approximate value to I in 56 significant digits, namely, about 16 significant digits are lost.

A Octuple precision system in C++

In this appendix we briefly show the octuple precision system, (called 'octo system'), in C++ due to Ninomiya. A floating point number R is expressed by a class constructor consisting of eight 4-byte unsigned integers defined by #typedef unsigned ul8[8]; the first bit for the sign S followed by 15 bits for the exponent E in the first element ul8[0] followed by remaining 16 bits of ul8[0] combined with the remaining 7 elements ul8[1],. . . ,ul8[7] for the mantissa M of total 240 bits, namely

$$R = (-1)^S (1 + M) \times 2^{(E-16383)}.$$

The floating point numbers in the octo system could express real numbers in more than 72 significant digits.

The octo system provides the facilities of the addition, subtraction, multiplication and division among two octo real numbers as well as octo complex numbers. Available are 72 functions including standard mathematical functions such as sinusoidal functions as well as special functions. Some important constants like π and table functions such as the zeta function $\zeta(n)$ and the Bernoulli number B_n are also available.

References

[1] M. Abramowitz, I. A. Stegun, Handbook of Mathematical Functions, Dover, NY (1972).

[2] F. Bornemann, D. Laurie, S. Wagon, J. Waldvogel, The SIAM 100-digit challenge: A study in high-accuracy numerical computing, SIAM, PA (2004).

[3] C. Brezinski, M. R. Zaglia, Extrapolation Methods, Theory and Practice, Elsevier, Amsterdam (1991).

[4] T. O. Espelid, Computation of an infinite integral using series acceleration, Numerical Algorithms, 40, 17–22 (2005).

[5] G. Evans, Practical Numerical Integration, John Wiley & Sons, NY (1993).

[6] W. Gautschi, The numerical evaluation of a challenging integral, Numerical Algorithms, DOI 10.1007/s11075-008-9157-z, (2008).

[7] É, Goursat, Cours d'Analyse Mathématique, tome 1, Gauthier Villars, Paris (1902).

[8] É, Goursat, A Course in Mathematical Analysis translated by O. Dunkel, E. R. Hedrick, Ginn, Boston (1904).

[9] G. H. Hardy, Mathematical Messenger, XXXI (1902).

[10] P. Henrici, Applied and Complex Analysis, Vol.1, John Wiley & Sons, NY (1974).

[11] I. Ninomiya, Improvement of adaptive Newton-Cotes quadrature methods, J. Inf. Process., 3, 162–170 (1980).

[12] I. Ninomiya, On a numerical integration by using an acceleration method, Kokyuroku, RIMS, Kyoto Univ., 585, 223-238 (1986) (in Japanese).

[13] A. Sidi, Practical Extrapolation Methods, Theory and Applications, Cambridge University Press (2003).

[14] M. Slevinsky, H. Safouhi, Numerical treatment of a twisted tail using extrapolation methods, Numerical Algorithms, 48, 301–316 (2008).

[15] H. Takahasi, M. Mori, Double exponential formulas for numerical integration, Publ. RIMS, Kyoto Univ., 9, 721–741 (1974).