High-Precision Numerical Integration and Experimental Mathematics

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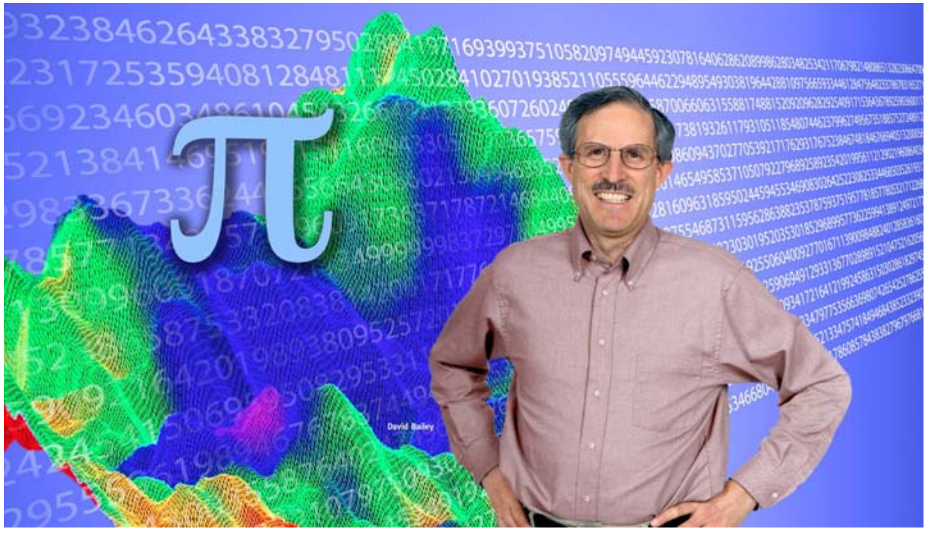
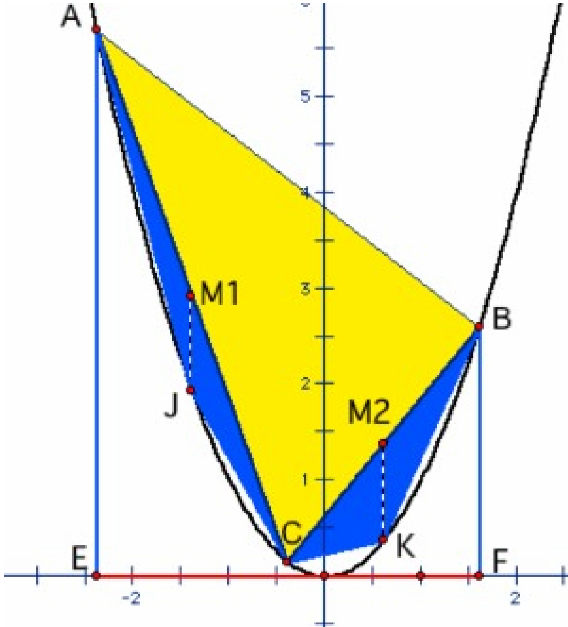


Historical Roots of Numerical Integration



- Archimedes (~ 225 BC) constructed an infinite sequence of triangles about a parabola, starting with one of area *A* of the same base and vertex, to obtain the areas

  $A, \; A + A/4, \; A + A/4 + A/16, \; A + A/4 + A/16 + A/64, \; \ldots$

  The area of the segment of the parabola is therefore

  $(1 + 1/4 + 1/16 + 1/64 + \ldots.)A = (4/3)A$.

- Archimedes used a similar "method of exhaustion" to find the area of a circle, thus yielding the first good approximate value of pi.

- Other "integrations" by Archimedes:
  - Volume and surface area of a sphere.
  - Volume and area of a cone.
  - Surface area of an ellipse.
  - Volume of a segment of a paraboloid of revolution.

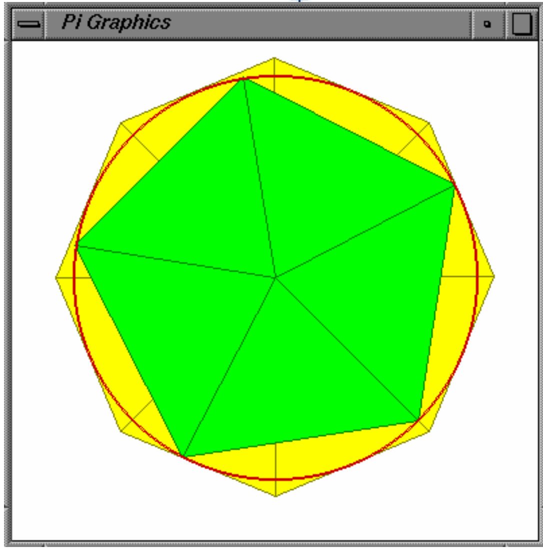


Illustration credits:

http://mtl.math.uiuc.edu/modules/module15/Unit%202/archim_ex.html
http://www.math.utah.edu/~alfeld/Archimedes/Archimedes.html

Quadrature (Numerical Integration) in the Computer Era

- Back in the 1960s and 1970s, Stenger, Schwartz and others observed that the trapezoidal rule can be used to formulate an efficient and accurate quadrature scheme, when combined with a transformation that converts the integrand function into a bell-shaped curve that goes to zero rapidly.
- One scheme discovered at the time is now known as the “tanh” rule.
- A related method is known as the “tanh-sinh” rule, which is now widely used in experimental mathematics.

Ref:

1. Frank Stenger, “Integration Formulae Based on the Trapezoidal Formula,” *Journal of the Institute for Mathematics and Applications*, vol. 12 (1973), pg. 103-114.
2. Charles Schwartz, “Numerical Integration of Analytic Functions,” *Journal of Computational Physics*, vol. 4 (1969), pg. 19-29.
3. H. Takahasi and M. Mori, “Double Exponential Formulas for Numerical Integration,” *Publications of RIMS*, Kyoto University, vol. 9 (1974), pg. 721--741.

The PSLQ Integer Relation Algorithm

Let (x_n) be a vector of real numbers. An integer relation algorithm finds integers (a_n) such that

$$a_1 x_1 + a_2 x_2 + \cdots + a_n x_n = 0$$

- At the present time, the PSLQ algorithm of mathematician-sculptor Helaman Ferguson is the best-known integer relation algorithm.
- PSLQ was named one of ten “algorithms of the century” by *Computing in Science and Engineering*.
- High-precision arithmetic software is required: at least d x n digits, where d is the size (in digits) of the largest of the integers a_k.

Refs:

1. H. R. P. Ferguson, D. H. Bailey and S. Arno, “Analysis of PSLQ, An Integer Relation Finding Algorithm,” *Mathematics of Computation*, vol. 68, no. 225 (Jan 1999), pg. 351-369.
2. D. H. Bailey and D. J. Broadhurst, “Parallel Integer Relation Detection: Techniques and Applications,” *Mathematics of Computation*, vol. 70, no. 236 (Oct 2000), pg. 1719-1736.

LBNL's Arbitrary Precision Software ARPREC and QD

- ARPREC: Arbitrary precision levels.
- QD: double-double (32 digits) and quad-double (64 digits).
- Written in C++ for performance and portability.
- C++ and Fortran-90 translation modules that permit conventional C++ and Fortran-90 programs to utilize the package with only very minor changes.
- High precision integer, floating and complex datatypes.
- Support for datatypes with differing precision levels.
- Common transcendental functions (exp, sin, log, erf, etc).
- Numerical integration routines.
- PSLQ routines.
- Special routines for extra-high precision (>1000 digits).

Available at: **`http://www.experimentalmath.info`**

The BBP Formula for Pi

In 1996, a computer program running the PSLQ algorithm discovered this formula for pi:

$$\pi = \sum_{k=0}^{\infty} \frac{1}{16^k} \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right)$$

This formula permits one to directly calculate binary or hexadecimal (base-16) digits of pi beginning at an arbitrary starting position n, without needing to calculate any of the first n-1 digits.

The discovery of this formula has led to several other results, including new results on the normality (digit randomness) of pi and log 2.

Ref:

1. D. H. Bailey, P. B. Borwein and S. Plouffe, “On the Rapid Computation of Various Polylogarithmic Constants,” *Mathematics of Computation*, vol. 66, no. 218 (Apr 1997), pg. 903-913.

Some Other Similar BBP-Type Identities

$$\pi^2 = \frac{1}{8}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{144}{(6k+1)^2}-\frac{216}{(6k+2)^2}-\frac{72}{(6k+3)^2}-\frac{54}{(6k+4)^2}+\frac{9}{(6k+5)^2}\right)$$

$$\pi^2 = \frac{2}{27}\sum_{k=0}^{\infty}\frac{1}{729^k}\left(\frac{243}{(12k+1)^2}-\frac{405}{(12k+2)^2}-\frac{81}{(12k+4)^2}-\frac{27}{(12k+5)^2}\right.$$
$$\left.-\frac{72}{(12k+6)^2}-\frac{9}{(12k+7)^2}-\frac{9}{(12k+8)^2}-\frac{5}{(12k+10)^2}+\frac{1}{(12k+11)^2}\right)$$

$$\zeta(3) = \frac{1}{1792}\sum_{k=0}^{\infty}\frac{1}{2^{12k}}\left(\frac{6144}{(24k+1)^3}-\frac{43008}{(24k+2)^3}+\frac{24576}{(24k+3)^3}+\frac{30720}{(24k+4)^3}\right.$$
$$-\frac{1536}{(24k+5)^3}+\frac{3072}{(24k+6)^3}+\frac{768}{(24k+7)^3}-\frac{3072}{(24k+9)^3}-\frac{2688}{(24k+10)^3}$$
$$-\frac{192}{(24k+11)^3}-\frac{1536}{(24k+12)^3}-\frac{96}{(24k+13)^3}-\frac{672}{(24k+14)^3}-\frac{384}{(24k+15)^3}$$
$$+\frac{24}{(24k+17)^3}+\frac{48}{(24k+18)^3}-\frac{12}{(24k+19)^3}+\frac{120}{(24k+20)^3}+\frac{48}{(24k+21)^3}$$
$$\left.-\frac{42}{(24k+22)^3}+\frac{3}{(24k+23)^3}\right)$$

$$\frac{25}{2}\log\left(\frac{781}{256}\left(\frac{57-5\sqrt{5}}{57+5\sqrt{5}}\right)^{\sqrt{5}}\right) = \sum_{k=0}^{\infty}\frac{1}{5^{5k}}\left(\frac{5}{5k+2}+\frac{1}{5k+3}\right)$$

Ref: Various papers by D. H. Bailey, P. B. Borwein, S. Plouffe, D. Broadhurst and R. E. Crandall.

Is There a Base-10 Formula for Pi?

For some constants, both a base-2 and a base-3 formula are known.

Question: Is there any base-n ($n \neq 2^b$) BBP-type formula for pi?
Answer: No. This is ruled out in a 2004 paper.

This does not rule out some completely different scheme for computing non-binary digits of pi beginning at an arbitrary starting point.

Ref: J. M. Borwein, W. F. Galway and D. Borwein, "Finding and Excluding b-ary Machin-Type BBP Formulae," *Canadian Journal of Mathematics*, vol. 56 (2004), pg 1339-1342.

Sample of Recent PSLQ Results: Euler Sum Identities

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2\frac{1}{(k+1)^4} \;=\; \frac{37}{22680}\pi^6-\zeta^2(3),$$

$$\sum_{n=1}^{\infty}\left(1+\frac{1}{2}+\frac{1}{3}+\cdots+\frac{1}{n}\right)^4\frac{1}{(n+1)^5} \;=$$

$$-\frac{29}{2}\zeta(9)+\frac{37}{2}\zeta(4)\zeta(5)+\frac{33}{4}\zeta(3)\zeta(6)-\frac{8}{3}\zeta^3(3)-7\zeta(2)\zeta(7),$$

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^3\frac{1}{(k+1)^6} \;=$$

$$\zeta^3(3)+\frac{197}{24}\zeta(9)+\frac{1}{2}\pi^2\zeta(7)-\frac{11}{120}\pi^4\zeta(5)-\frac{37}{7560}\pi^6\zeta(3).$$

Ref: David H. Bailey, Jonathan M. Borwein and Roland Girgensohn, "Experimental Evaluation of Euler Sums", Experimental Mathematics, vol. 3, no. 1 (1994), pg. 17-30.

Sample of Recent PSLQ Results: Apery-Like Sum Identities

The following identities were recently found using integer relation methods:

$$
\begin{aligned}
\zeta(5) &= 2\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}} - \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2},\\
\zeta(7) &= \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}} + \frac{25}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\\
\zeta(9) &= \frac{9}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^9\binom{2k}{k}} - \frac{5}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^7\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^2} + 5\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^5\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\\
&\quad + \frac{45}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^6} - \frac{25}{4}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}}\sum_{j=1}^{k-1}\frac{1}{j^4}\sum_{j=1}^{k-1}\frac{1}{j^2},\\
\sum_{n=0}^{\infty}\zeta(4n+3)x^{4n} &= \frac{5}{2}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^3\binom{2k}{k}(1-x^4/k^4)}\prod_{m=1}^{k-1}\left(\frac{1+4x^4/m^4}{1-x^4/m^4}\right)\\
\sum_{n=0}^{\infty}\zeta(2n+2)x^{2n} &= 3\sum_{k=1}^{\infty}\frac{1}{k^2\binom{2k}{k}\left(1-x^2/k^2\right)}\prod_{m=1}^{k-1}\left(\frac{1-4\,x^2/m^2}{1-x^2/m^2}\right)
\end{aligned}
$$

Ref: D. H. Bailey, J. M. Borwein and D. M. Bradley, "Experimental Determination of Apery-Like Identities for Zeta(2n+2)," *Experimental Mathematics*, vol. 15 (2006), pg. 281-289 .

The Euler-Maclaurin Formula of Numerical Analysis

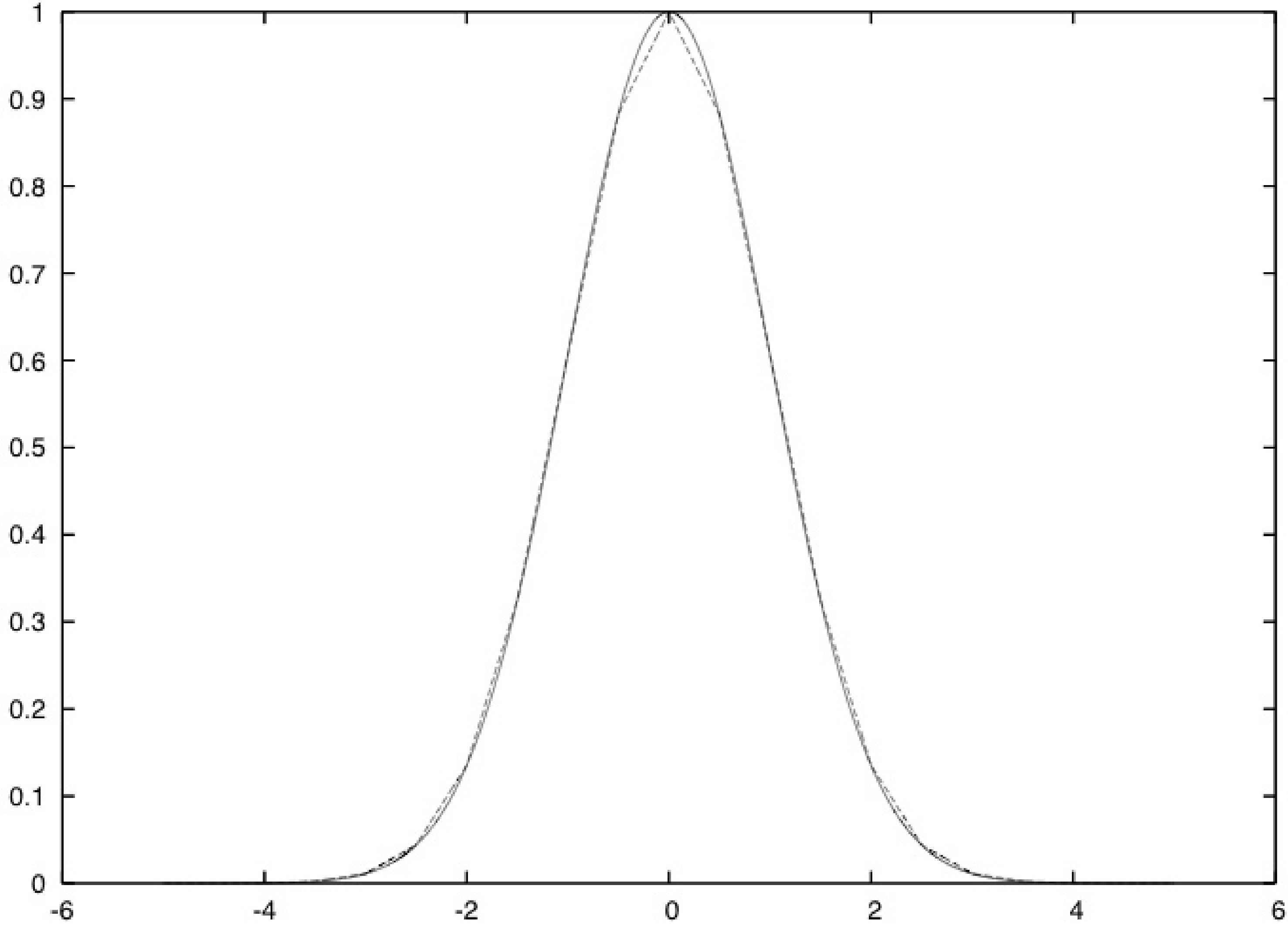
$$
\begin{aligned}
\int_a^b f(x)\,dx &= h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}(f(a)+f(b)) \\
&- \sum_{i=1}^{m} \frac{h^{2i}B_{2i}}{(2i)!}\left(f^{(2i-1)}(b) - f^{(2i-1)}(a)\right) - E(h) \\
|E(h)| &\le 2(b-a)[h/(2\pi)]^{2m+2} \max_{a\le x\le b} |D^{2m+2}f(x)|
\end{aligned}
$$

[Here $h = (b - a)/n$ and $x_j = a + j\,h$. $D^m f(x)$ means m-th derivative of f.]

Note when f(t) and all of its derivatives are zero at a and b (as in a bell-shaped curve), the error E(h) of a simple trapezoidal approximation to the integral goes to zero more rapidly than any power of h.

Ref: Kendall Atkinson, *An Introduction to Numerical Analysis*, John Wiley, 1989, pg. 289.

Trapezoidal Approximation to a Bell-Shaped Function



High-Precision Integration and the Euler-Maclaurin Formula

Given f(x) defined on (-1,1), employ a function g(t) that goes from -1 to 1 over the real line, with g'(t) going to zero for large |t|. Then setting x = g(t) yields

$$\int_{-1}^{1} f(x)\,dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\,dt \;\approx\; h\sum_{-N}^{N} w_j f(x_j)$$

Here x_j = g(hj) and w_j = g'(hj). If g'(t) goes to zero rapidly enough for large t, then even if f(x) has a vertical derivative or blow-up singularity at an endpoint, the product f(g(t)) g'(t) typically is a nice bell-shaped function for which the E-M formula applies.

Such schemes often achieve quadratic convergence – reducing h by half produces twice as many correct digits.

Ref: David H. Bailey, Xiaoye S. Li and Karthik Jeyabalan, "A Comparison of Three High-Precision Quadrature Schemes," *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317-329.

Four Suitable ‘g’ Functions

$$g(t) = \mathrm{erf}(t) \qquad g'(t) = \frac{2}{\sqrt{\pi}} e^{-t^2}$$

$$g(t) = \tanh t \qquad g'(t) = \frac{1}{\cosh^2 t}$$

$$g(t) = \tanh(\sinh t) \qquad g'(t) = \frac{\sinh t}{\cosh^2(\sinh t)}$$

$$g(t) = \tanh(\pi/2 \cdot \sinh t) \qquad g'(t) = \frac{\pi/2 \cdot \sinh t}{\cosh^2(\pi/2 \cdot \sinh t)}$$

“Error function” or “Erf” quadrature uses the first formula.

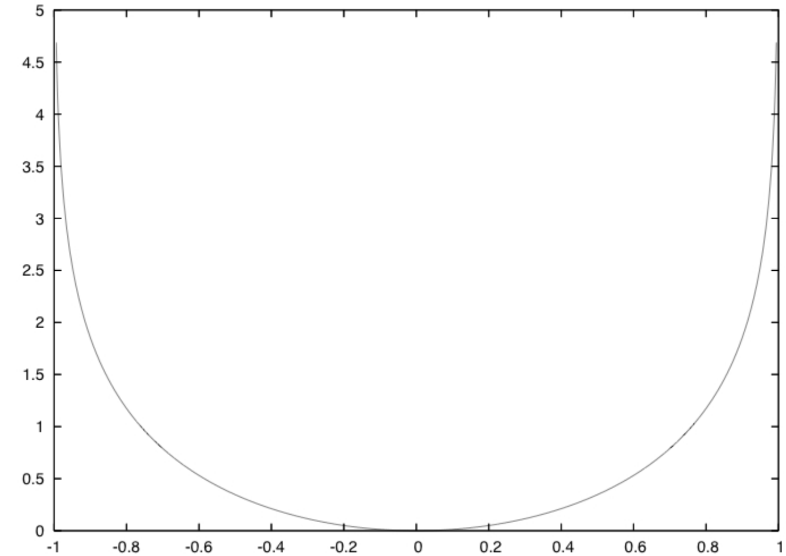
“Tanh” quadrature uses the second formula.

“Tanh-sinh” quadrature uses one of the last two formulas.

Original and Transformed Integrand Functions

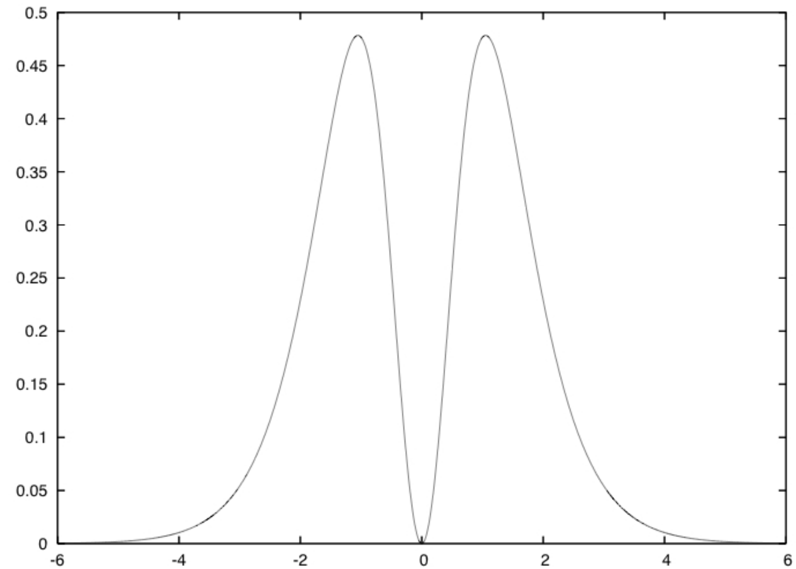
Original function on [-1,1]:

$$f(t) \quad = \quad -\log\cos\left(\frac{\pi t}{2}\right)$$



Transformed function on real line using tanh rule:

$$f(g(t))g'(t) \quad = \quad -\frac{2}{\sqrt{\pi}}\log\cos\left(\frac{\pi\tanh t}{2}\right)/\cosh^2 t$$



Gaussian Quadrature Versus Tanh-Sinh Quadrature

Gaussian quadrature:

- Most efficient scheme for continuous, well-behaved functions.
- In many cases, halving the integration interval doubles the number of correct digits in the result.
- Performs poorly for functions with blow-up singularities or vertical derivatives at endpoints.
- The cost of computing abscissas and weights increases as n^2 and thus becomes impractical for use beyond a few hundred digits.

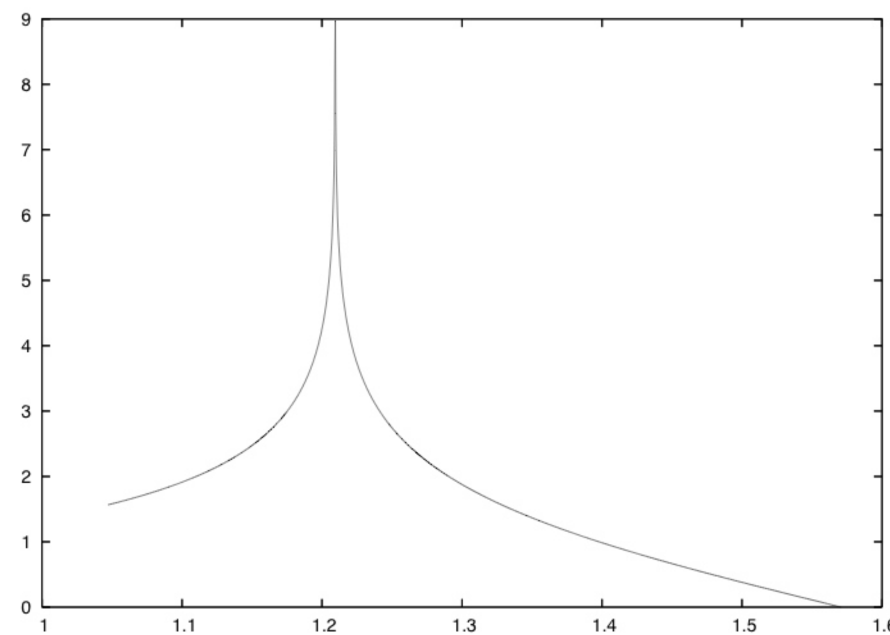
Tanh-sinh quadrature:

- Accurately evaluates almost all “reasonable” functions, even those with singularities or vertical derivatives at endpoints.
- In many cases, halving the integration interval doubles the number of correct digits in the result.
- The cost of computing abscissas and weights increases only as n, so the scheme is suitable for hundreds or thousands of digits.

Application of High-Precision Tanh-Sinh Quadrature

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt$$
$$\stackrel{?}{=} \sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2} \right]$$

This arises from analysis of volumes of ideal tetrahedra in hyperbolic space. This “identity” has now been verified numerically to 20,000 digits, but no proof is known.



Ref: D.H. Bailey, J.M. Borwein, V. Kapoor and E. Weisstein, “Ten Problems in Experimental Mathematics,” *Am. Math. Monthly*, Jun 2006.

Box Integrals

Spurred by a question posed in Jan 2006 by Luis Goddyn of SFU, we examined integrals of the form:

$$B_n(s) = \int_0^1 \cdots \int_0^1 \left(r_1^2 + \ldots + r_n^2\right)^{s/2} \, dr_1 \cdots dr_n$$

The following evaluations are now known:

$$B_1(1) = \frac{1}{2}$$

$$B_2(1) = \frac{\sqrt{2}}{3} + \frac{1}{3} \log\left(\sqrt{2}+1\right)$$

$$B_3(1) = \frac{\sqrt{3}}{4} + \frac{1}{2} \log\left(2+\sqrt{3}\right) - \frac{\pi}{24}$$

$$B_4(1) = \frac{2}{5} + \frac{7}{20}\pi\sqrt{2} - \frac{1}{20}\pi \log\left(1+\sqrt{2}\right) + \log(3) - \frac{7}{5}\sqrt{2}\arctan\left(\sqrt{2}\right) + \frac{1}{10}\mathcal{K}_0$$

where

$$\mathcal{K}_0 = \int_0^1 \frac{\log(1+\sqrt{3+y^2}) - \log(-1+\sqrt{3+y^2})}{1+y^2} \, dy$$

Ref: D. H. Bailey, J. M. Borwein and R. E. Crandall, “Box Integrals,” *Journal of Computational and Applied Mathematics*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/boxintegrals.pdf.

Ising Integrals

We recently applied our methods to study three classes of integrals that arise in the Ising theory of mathematical physics:

$$C_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$D_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \frac{\prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2}{\left(\sum_{j=1}^n (u_j + 1/u_j)\right)^2} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

$$E_n := \frac{4}{n!}\int_0^\infty \cdots \int_0^\infty \prod_{i<j}\left(\frac{u_i-u_j}{u_i+u_j}\right)^2 \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

Ref: David H. Bailey, Jonathan M. Borwein and Richard E. Crandall, “Integrals of the Ising Class,” *Journal of Physics A: Mathematical and General*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/ising.pdf.

Computing and Evaluating C_n

Richard Crandall showed that the multi-dimensional C_n integrals can be transformed to 1-D integrals:

$$C_n = \frac{2^n}{n!} \int_0^\infty t K_0^n(t)\ dt$$

where K_0 is the modified Bessel function.

We used this formula to compute 1000-digit numerical values of various C_n, from which these results and others were found (and subsequently proven):

$$\begin{aligned}
C_1 &= 2 \\
C_2 &= 1 \\
C_3 &= \mathrm{L}_{-3}(2) = \sum_{n \ge 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right) \\
C_4 &= 14\zeta(3)
\end{aligned}$$

Limiting Value of C_n

The C_n numerical values approach a limit:

$$
\begin{aligned}
C_{10} &= 0.63188002414701222229035087366080283... \\
C_{40} &= 0.63047350337836353186994190185909694... \\
C_{100} &= 0.63047350337438679612204019271903171... \\
C_{200} &= 0.63047350337438679612204019271087890...
\end{aligned}
$$

What is this limit? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator tool, available at

`http://oldweb.cecm.sfu.ca/projects/ISC/ISCmain.html`

The result was: $2e^{-2\gamma}$

where gamma denotes Euler's constant.

Limiting Value of C_n

We can prove this limit, and obtain a high-order expansion by writing

$$C_n = \frac{2^n}{n!}\left(\int_0^{p_0} + \int_{p_0}^{\infty}\right) p K_0^n(p)\; dp = \frac{2^n}{n!}\int_0^{p_0} p\, K_0^n(p)\; dp + \Theta\left(\frac{1}{n!}\right)$$

where

$$p_0 = 2e^{-2\gamma}$$

By applying the well-known identity (here H_k is the harmonic number)

$$K_0(t) = \sum_{k\geq 0} \frac{t^{2k}}{4^k k!^2}\left(H_k - \left(\gamma + \log\frac{t}{2}\right)\right)$$

and applying various manipulations, we obtain

$$C_n = 2\,e^{-2\gamma} + \frac{n+4}{2^n}e^{-4\gamma} + \frac{2n^2+23n+57}{3^n \cdot 6}e^{-6\gamma} + \cdots$$

Other Evaluations

$$
\begin{aligned}
D_2 &= 1/3\\
D_3 &= 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2)\\
D_4 &= 4\pi^2/9 - 1/6 - 7\zeta(3)/2\\
E_2 &= 6 - 8\log 2\\
E_3 &= 10 - 2\pi^2 - 8\log 2 + 32\log^2 2\\
E_4 &= 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3\\
&\quad +16\pi^2\log 2 - 22\pi^2/3\\
E_5 &\stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2\\
&\quad +40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2\\
&\quad +464\log^2 2 - 40\log 2
\end{aligned}
$$

The Ising Integral E_5

We were able to reduce E_5, which is a 5-D integral, to an extremely complicated 3-D integral (see below).

We computed this integral to 250-digit precision, using a parallel high-precision 3-D quadrature program. Then we used a PSLQ program to discover the evaluation given on the previous page.

$$
\begin{aligned}
E_5 = \int_0^1\int_0^1\int_0^1 & [2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 (-[4(x+1)(xy+1)\log(2)(y^5z^3x^7-y^4z^2(4(y+1)z+3)x^6-y^3z((y^2+1)z^2+4(y+ \\
& 1)z+5)x^5+y^2(4y(y+1)z^3+3(y^2+1)z^2+4(y+1)z-1)x^4+y(z(z^2+4z+5)y^2+4(z^2+1)y+5z+4)x^3+((-3z^2-4z+1)y^2-4zy+1)x^2 \\
& -(y(5z+4)+4)x-1)]/[(x-1)^3(xy-1)^3(xyz-1)^3]+[3(y-1)^2y^4(z-1)^2z^2(yz-1)^2x^6+2y^3z(3(z-1)^2z^3y^5+z^2(5z^3+3z^2+3z+5)y^4+(z-1)^2z \\
& (5z^2+16z+5)y^3+(3z^5+3z^4-22z^3-22z^2+3z+3)y^2+3(-2z^4+z^3+2z^2+z-2)y+3z^3+5z^2+5z+3)x^5+y^2(7(z-1)^2z^4y^6-2z^3(z^3+15z^2 \\
& +15z+1)y^5+2z^2(-21z^4+6z^3+14z^2+6z-21)y^4-2z(z^5-6z^4-27z^3-27z^2-6z+1)y^3+(7z^6-30z^5+28z^4+54z^3+28z^2-30z+7)y^2-2(7z^5 \\
& +15z^4-6z^3-6z^2+15z+7)y+7z^4-2z^3-42z^2-2z+7)x^4-2y(z^3(z^3-9z^2-9z+1)y^6+z^2(7z^4-14z^3-18z^2-14z+7)y^5+z(7z^5+14z^4+3 \\
& z^3+3z^2+14z+7)y^4+(z^6-14z^5+3z^4+84z^3+3z^2-14z+1)y^3-3(3z^5+6z^4-z^3-z^2+6z+3)y^2-(9z^4+14z^3-14z^2+14z+9)y+z^3+7z^2+7z \\
& +1)x^3+(z^2(11z^4+6z^3-66z^2+6z+11)y^6+2z(5z^5+13z^4-2z^3-2z^2+13z+5)y^5+(11z^6+26z^5+44z^4-66z^3+44z^2+26z+11)y^4+(6z^5-4 \\
& z^4-66z^3-66z^2-4z+6)y^3-2(33z^4+2z^3-22z^2+2z+33)y^2+(6z^3+26z^2+26z+6)y+11z^2+10z+11)x^2-2(z^2(5z^3+3z^2+3z+5)y^5+z(22z^4 \\
& +5z^3-22z^2+5z+22)y^4+(5z^5+5z^4-26z^3-26z^2+5z+5)y^3+(3z^4-22z^3-26z^2-22z+3)y^2+(3z^3+5z^2+5z+3)y+5z^2+22z+5)x+15z^2+2z \\
& +2y(z-1)^2(z+1)+2y^3(z-1)^2z(z+1)+y^4z^2(15z^2+2z+15)+y^2(15z^4-2z^3-90z^2-2z+15)+15]/[(x-1)^2(y-1)^2(xy-1)^2(z-1)^2(yz-1)^2 \\
& (xyz-1)^2]-[4(x+1)(y+1)(yz+1)(-z^2y^4+4z(z+1)y^3+(z^2+1)y^2-4(z+1)y+4x(y^2-1)(y^2z^2-1)+x^2(z^2y^4-4z(z+1)y^3-(z^2+1)y^2 \\
& +4(z+1)y+1)-1)\log(x+1)]/[(x-1)^3x(y-1)^3(yz-1)^3]-[4(y+1)(xy+1)(z+1)(x^2(z^2-4z-1)y^4+4x(x+1)(z^2-1)y^3-(x^2+1)(z^2-4z-1) \\
& y^2-4(x+1)(z^2-1)y+z^2-4z-1)\log(xy+1)]/[x(y-1)^3y(xy-1)^3(z-1)^3]-[4(z+1)(yz+1)(x^3y^5z^7+x^2y^4(4x(y+1)+5)z^6-xy^3((y^2+ \\
& 1)x^2-4(y+1)x-3)z^5-y^2(4y(y+1)x^3+5(y^2+1)x^2+4(y+1)x+1)z^4+y(y^2x^3-4y(y+1)x^2-3(y^2+1)x-4(y+1))z^3+(5x^2y^2+y^2+4x(y+1) \\
& y+1)z^2+((3x+4)y+4)z-1)\log(xyz+1)]/[xy(z-1)^3z(yz-1)^3(xyz-1)^3])]/[(x+1)^2(y+1)^2(xy+1)^2(z+1)^2(yz+1)^2(xyz+1)^2] \\
& dx\,du\,dz
\end{aligned}
$$

Recursions in Ising Integrals

Consider this 2-parameter class of Ising integrals:

$$C_{n,k} = \frac{4}{n!} \int_0^\infty \cdots \int_0^\infty \frac{1}{\left(\sum_{j=1}^{n}(u_j + 1/u_j)\right)^{k+1}} \frac{du_1}{u_1} \cdots \frac{du_n}{u_n}$$

After computing 1000-digit numerical values for all n up to 36 and all k up to 75 (a total of 2660 individual quadrature calculations), we discovered (using PSLQ) linear relations in the rows of this array. For example, when n = 3:

$$\begin{aligned}
0 &= C_{3,0} - 84C_{3,2} + 216C_{3,4} \\
0 &= 2C_{3,1} - 69C_{3,3} + 135C_{3,5} \\
0 &= C_{3,2} - 24C_{3,4} + 40C_{3,6} \\
0 &= 32C_{3,3} - 630C_{3,5} + 945C_{3,7} \\
0 &= 125C_{3,4} - 2172C_{3,6} + 3024C_{3,8}
\end{aligned}$$

Similar, but more complicated, recursions were found for larger n (next page).

Ref: David H. Bailey, David Borwein, Jonathan M. Borwein and Richard Crandall, “Hypergeometric Forms for Ising-Class Integrals,” *Experimental Mathematics*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/meijer/pdf.

Experimental Recursion for n = 24

$$
\begin{aligned}
0 \stackrel{?}{=} \; & C_{24,1} \\
& -1107296298\, C_{24,3} \\
& +128857433617566 0\, C_{24,5} \\
& -88962910652291256000\, C_{24,7} \\
& +1211528914846561331193600\, C_{24,9} \\
& -5367185923241422152980553600\, C_{24,11} \\
& +9857686103738772925980190636800\, C_{24,13} \\
& -8476778037073141951236532459008000\, C_{24,15} \\
& +3590120926882411593645052529049600000\, C_{24,17} \\
& -745759114781380983188217871663104000000\, C_{24,19} \\
& +71215552121869985477578381170258739200000\, C_{24,21} \\
& -2649853457247995406113355087174696960000000\, C_{24,23} \\
& +24912519234220575094208313195233280000000000\, C_{24,25}
\end{aligned}
$$

General Recursion Formulas

We were able to find general recursion formulas for each n up to 36:

$$
\begin{aligned}
0 &= (k+1)C_{1,k} - (k+2)C_{1,k+2} \\
0 &= (k+1)^2 C_{2,k} - 4(k+2)^2 C_{2,k+2} \\
0 &= (k+1)^3 C_{3,k} - 2(k+2)\left(5(k+2)^2+1\right) C_{3,k+2} \\
&\quad +9(k+2)(k+3)(k+4)C_{3,k+4} \\
0 &= (k+1)^4 C_{4,k} - 4(k+2)^2(5(k+2)^2+3)C_{4,k+2} \\
&\quad +64(k+2)(k+3)^2(k+4)C_{4,k+4} \\
0 &\stackrel{?}{=} (k+1)^5 C_{5,k} - (k+2)\left(35k^4+280k^3+882k^2+1288k+731\right) C_{5,k+2} \\
&\quad +(k+2)(k+3)(k+4)\left(259k^2+1554k+2435\right) C_{5,k+4} \\
&\quad -225(k+2)(k+3)(k+4)(k+5)(k+6)C_{5,k+6}
\end{aligned}
$$

New Result: A new manuscript by Jonathan Borwein and Bruno Salvy proves that the Cn,k satisfy recursions. The authors hope to rigorously establish all of the experimental results mentioned here.

Spin Integrals

In another application of experimental high-precision integration to mathematical physics, we recently investigated some integrals first studied by Boos and Korepin:

$$P(n) = \frac{1}{(2\pi i)^n} \int_{\mathcal{C}^n} U_n T_n \, d\lambda_1 \, d\lambda_2 \cdots d\lambda_n$$

Here C denotes the contour {x - i/2, x on real line}, and

$$U_n = \pi^{n(n+1)/2} \cdot \frac{\prod_{j<k} \sinh \pi(\lambda_k - \lambda_j)}{\prod_j \sinh^n \pi \lambda_j}$$

$$T_n = \frac{\prod_j \lambda_j^{j-1} (\lambda_j + i)^{n-j}}{\prod_{j<k} (\lambda_k - \lambda_j - i)}$$

Ref: D. H. Bailey, J. M. Borwein, R. E. Crandall, D. Manna, “New Representations for Spin Integrals,” manuscript, 2007 (work in progress).

Spin Integrals

We were able to transform this expression to the following more manageable form over a finite n-dimensional interval:

$$P(n) = \frac{(-1)^{\lfloor n/2 \rfloor}}{(2\pi)^n} \int_{-\pi/2}^{\pi/2} \cdots \int_{-\pi/2}^{\pi/2} \prod_j \left(a_j - \frac{i\pi}{2}\right)^{j-1} \left(a_j + \frac{i\pi}{2}\right)^{n-j}$$

$$\times \prod_{1 \le k < h \le n} \frac{\sin \phi_h - \sin \phi_k}{a_h - a_k - i\pi} \, d\phi_1 \, d\phi_2 \cdots d\phi_n$$

By evaluating this n-dimensional integral numerically, we have verified some analytic evaluations given by Boos and Korepin, and hope to extend their results.

Evaluations of P(n)
Derived Analytically, Confirmed Numerically

$$
\begin{aligned}
P(2) &= \frac{1}{3} - \frac{1}{3}\log 2 \\
P(3) &= \frac{1}{4} - \log 2 + \frac{3}{8}\zeta(3) \\
P(4) &= \frac{1}{5} - 2\log 2 + \frac{173}{60}\zeta(3) - \frac{11}{6}\zeta(3)\log 2 - \frac{51}{80}\zeta^2(3) - \frac{55}{24}\zeta(5) \\
&\quad + \frac{85}{24}\zeta(5)\log 2 \\
P(5) &= \frac{1}{6} - \frac{10}{3}\log 2 + \frac{281}{24}\zeta(3) - \frac{45}{2}\zeta(3)\log 2 - \frac{489}{16}\zeta^2(3) \\
&\quad - \frac{6775}{192}\zeta(5) + \frac{1225}{6}\zeta(5)\log 2 - \frac{425}{64}\zeta(3)\zeta(5) - \frac{12125}{256}\zeta^2(5) \\
&\quad + \frac{6223}{256}\zeta(7) - \frac{11515}{64}\zeta(7)\log 2 + \frac{42777}{512}\zeta(3)\zeta(7)
\end{aligned}
$$

Evaluation of P(6)

$$
\begin{aligned}
P(6) \;=\; \frac{1}{7}\Big[& 1 - 35\eta(1) + 322\eta(3) - \frac{9244}{5}\eta(5) + \frac{22694}{5}\eta(7) - 2982\eta(9) \\
& - \frac{3920}{3}\eta(1)\eta(3) + \frac{369908}{15}\eta(1)\eta(5) - \frac{28784}{5}\eta^2(3) - \frac{263816}{3}\eta(1)\eta(7) \\
& + \frac{3458}{15}\eta(3)\eta(5) + \frac{323344}{5}\eta(1)\eta(9) + \frac{933702}{5}\eta(3)\eta(7) - \frac{751592}{9}\eta^2(5) \\
& - \frac{2627842}{15}\eta(3)\eta(9) + \frac{235963}{9}\eta(5)\eta(7) + \frac{368564}{3}\eta(5)\eta(9) - \frac{644987}{9}\eta^2(7) \\
& + \frac{538496}{45}\eta(1)\eta(3)\eta(5) - \frac{269248}{135}\eta^3(3) - \frac{1143268}{9}\eta(1)\eta(3)\eta(7) \\
& + \frac{653296}{9}\eta(1)\eta^2(5) - \frac{163324}{45}\eta^2(3)\eta(5) + \frac{1737148}{15}\eta(1)\eta(3)\eta(9) \\
& - \frac{1737148}{45}\eta^2(3)\eta(7) + \frac{124082}{9}\eta(3)\eta^2(5) - \frac{528164}{3}\eta(1)\eta(5)\eta(9) \\
& + \frac{924287}{9}\eta(1)\eta^2(7) + \frac{264082}{5}\eta^2(3)\eta(9) - \frac{264082}{9}\eta(3)\eta(5)\eta(7) \\
& + \frac{188630}{27}\eta^3(5)\Big]
\end{aligned}
$$

where

$$\eta(m) \;=\; (1 - 2^{1-m})\zeta(m)$$

Computation Time for P(n)

- P(2): 120 digits in 10 seconds.
- P(3): 120 digits in 55 minutes on 8 CPUs.
- P(4): 60 digits in 27 minutes on 64 CPUs.
- P(5): 30 digits in 39 minutes on 256 CPUs.
- P(6): 6 digits in 59 hours on 256 CPUs.

We need new, more efficient techniques for evaluating multi-dimensional integrals!

Conclusions

- High-precision numerical integration has emerged as an extremely valuable tool in engineering, physics and experimental mathematics.
- The theoretical foundation for this work was laid down by Stenger, Schwarz and other pioneers in the 1960s and 1970s.
- Tanh-sinh quadrature, which derives from this early work, is very robust and efficient, especially for integrands with singularities or vertical derivatives at endpoints, or for precision levels greater than 1000 digits.

But significant challenges remain:

- We need to better understand the behavior of these schemes across a wide range of integrand functions.
- Efficient, high-precision computation of multi-dimensional integrals, both for regular and non-regular integrands, remains a major challenge.
- Some completely new approaches to integration should be investigated.