High-Precision, High-Dimension Integration

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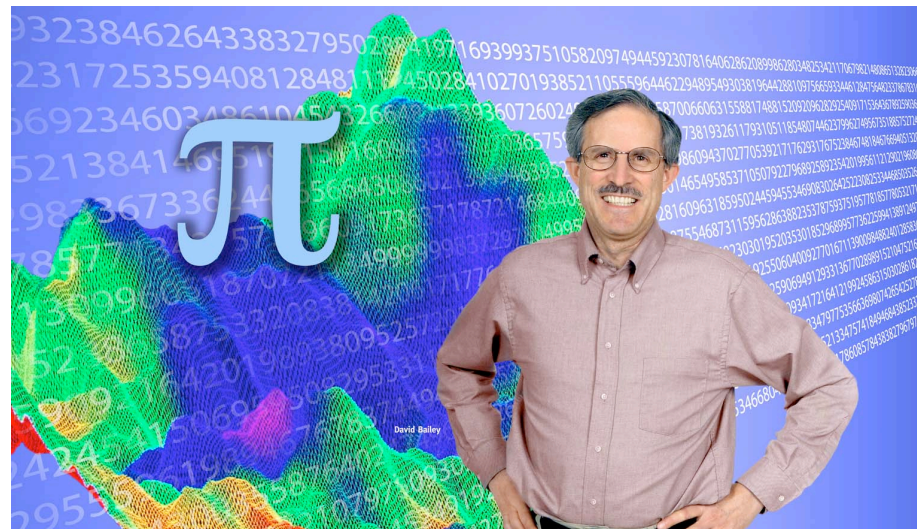
Applications of High-Precision Arithmetic in Modern Scientific Computing

- Highly nonlinear computations.
- Computations involving highly ill-conditioned linear systems.
- Computations involving data with very large dynamic range.
- Large computations on highly parallel computer systems.
- Computations where numerical sensitivity is not currently a major problem, but periodic testing is needed to ensure that results are reliable.
- Research problems in mathematics and mathematical physics that involve constant recognition and integer relation detection.

Few physicists, chemists or engineers are highly expert in numerical analysis. Thus high-precision arithmetic is often a better remedy for severe numerical round-off error, even if the error could, in principle, be improved with more advanced algorithms or coding techniques.

Consider the very simple differential equation $y''(x) = -f(x)$. Discretization leads to the matrix:

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 & 2 \end{bmatrix}$$
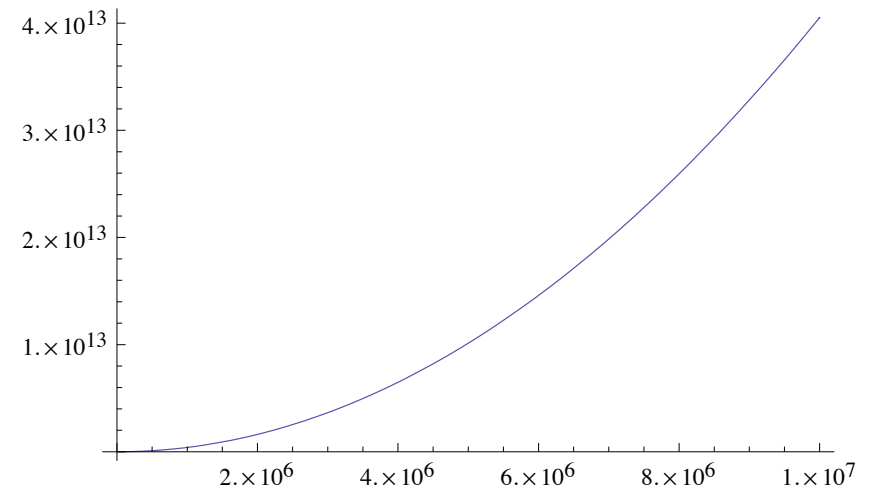
The condition number of this matrix (the quotient of the largest eigenvalue to the smallest eigenvalue) is readily seen to be approximately

$$\kappa(n) \approx \frac{4(n+1)^2}{\pi^2}$$

For modest-sized n, many systems of this type (depending on the right-hand side) cannot be reliably solved using 64-bit arithmetic.

Available High-Precision Facilities

Vendor-supported arithmetic:

Type	Total Bits	Significant Digits	Support
IEEE Double	64	16	In hardware on almost all systems.
IEEE Extended	80	18	In hardware on Intel and AMD systems.
IEEE Quad	128	33	In software from some vendors (50-100X slower than IEEE double).

Non-commercial (free) software:

Type	Total Bits	Significant Digits	Support
Double-double	128	32	DDFUN90, QD.
Quad-double	256	64	QD.
Arbitrary	Any	Any	ARPREC, MPFUN90, GMP, MPFR.

Commercial software: *Mathematica, Maple*.

LBNL's High-Precision Software
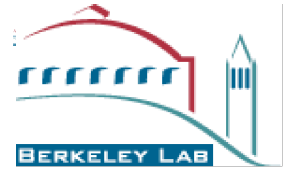
- QD: double-double (31 digits) and quad-double (62 digits).
- ARPREC: arbitrary precision.
- Low-level routines written in C++.
- C++ and Fortran-90 translation modules permit use with existing C++ and Fortran-90 programs -- only minor code changes are required.
- Includes many common functions: sqrt, cos, exp, gamma, etc.
- PSLQ, root finding, numerical integration.

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

Authors: Xiaoye Li, Yozo Hida, Brandon Thompson and DHB

GNU Multiprecision Library:

♦ High-level signed integer arithmetic functions (mpz).

♦ High-level rational arithmetic functions (mpq).

♦ High-level floating-point arithmetic functions (mpf).

♦ C++ class-based interface to all of the above.

Available at: http://gmplib.org/

MPFR:

♦ C library of floating-point accurately rounding arithmetic functions.

Available at: http://www.mpfr.org

C++ high-level interfaces based on MPFR:

♦ MPFRCPP

♦ MPFR++

♦ GMPFRXX

Some Real-World Applications of High-Precision Arithmetic

- Supernova simulations (32 or 64 digits).
- Climate modeling (32 digits).
- Planetary orbit calculations (32 digits).
- Coulomb n-body atomic system simulations (32-120 digits).
- Schrodinger solutions for lithium and helium atoms (32 digits).
- Electromagnetic scattering theory (32-100 digits).
- Studies of the fine structure constant of physics (32 digits).
- Scattering amplitudes of quarks, gluons and bosons (32 digits).
- Theory of nonlinear oscillators (64 digits).

Application of High-Precision Arithmetic: Supernova Simulations

♦ Researchers at LBNL are using QD to solve for non-local thermodynamic equilibrium populations of iron and other atoms in the atmospheres of supernovas.

♦ Iron may exist in several species, so it is necessary to solve for all species simultaneously.

♦ Since the relative population of any state from the dominant state is proportional to the exponential of the ionization energy, the dynamic range of these values can be very large.

♦ The quad-double portion now dominates the entire computation.
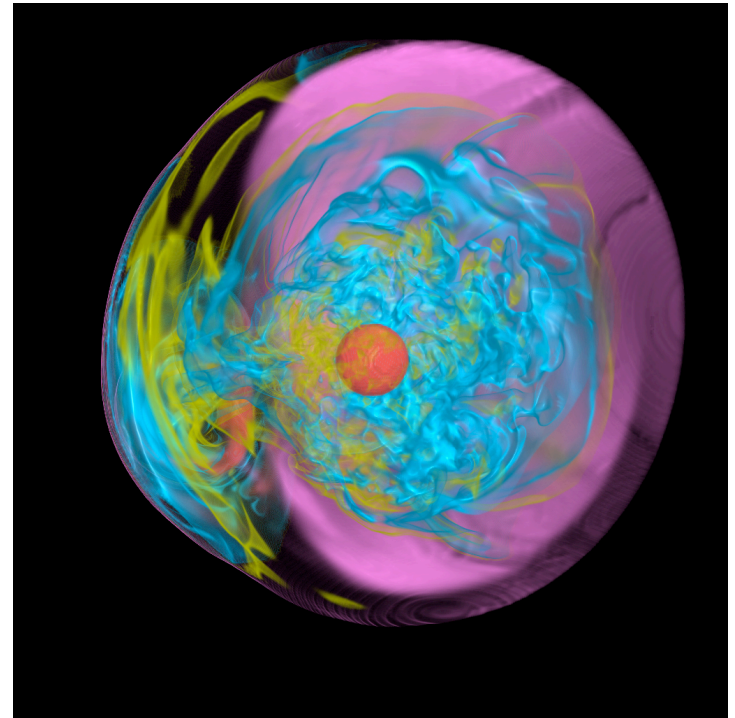
P. H. Hauschildt and E. Baron, "The Numerical Solution of the Expanding Stellar Atmosphere Problem," *Journal Computational and Applied Mathematics*, vol. 109 (1999), pg. 41-63.

Coulomb N-Body Atomic System Simulations

♦ Alexei Frolov of Queen's University in Canada has used MPFUN90 to solve a generalized eigenvalue problem that arises in Coulomb n-body interactions.

♦ Matrices are typically 5,000 x 5,000 and are very nearly singular.

♦ Frolov has also computed elements of the Hamiltonian matrix and the overlap matrix in four- and five-body systems.

♦ These computations typically require 120-digit arithmetic.

"We can consider and solve the bound state few-body problems which have been beyond our imagination even four years ago." – Frolov

A. M. Frolov and DHB, "Highly Accurate Evaluation of the Few-Body Auxiliary Functions and Four-Body Integrals," *Journal of Physics B*, vol. 36, no. 9 (14 May 2003), pg. 1857-1867.

The PSLQ Integer Relation Algorithm

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

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

(or within "epsilon" of zero, where epsilon = 10^{-p} and p is the precision).

At the present time the "PSLQ" algorithm of mathematician-sculptor Helaman Ferguson is the most widely used integer relation algorithm. It was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.

PSLQ (or any other integer relation scheme) requires very high precision (at least $n*d$ digits, where d is the size in digits of the largest a_k), both in the input data and in the operation of the algorithm.

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

Decrease of $\log_{10}(\min |x_i|)$ in PSLQ
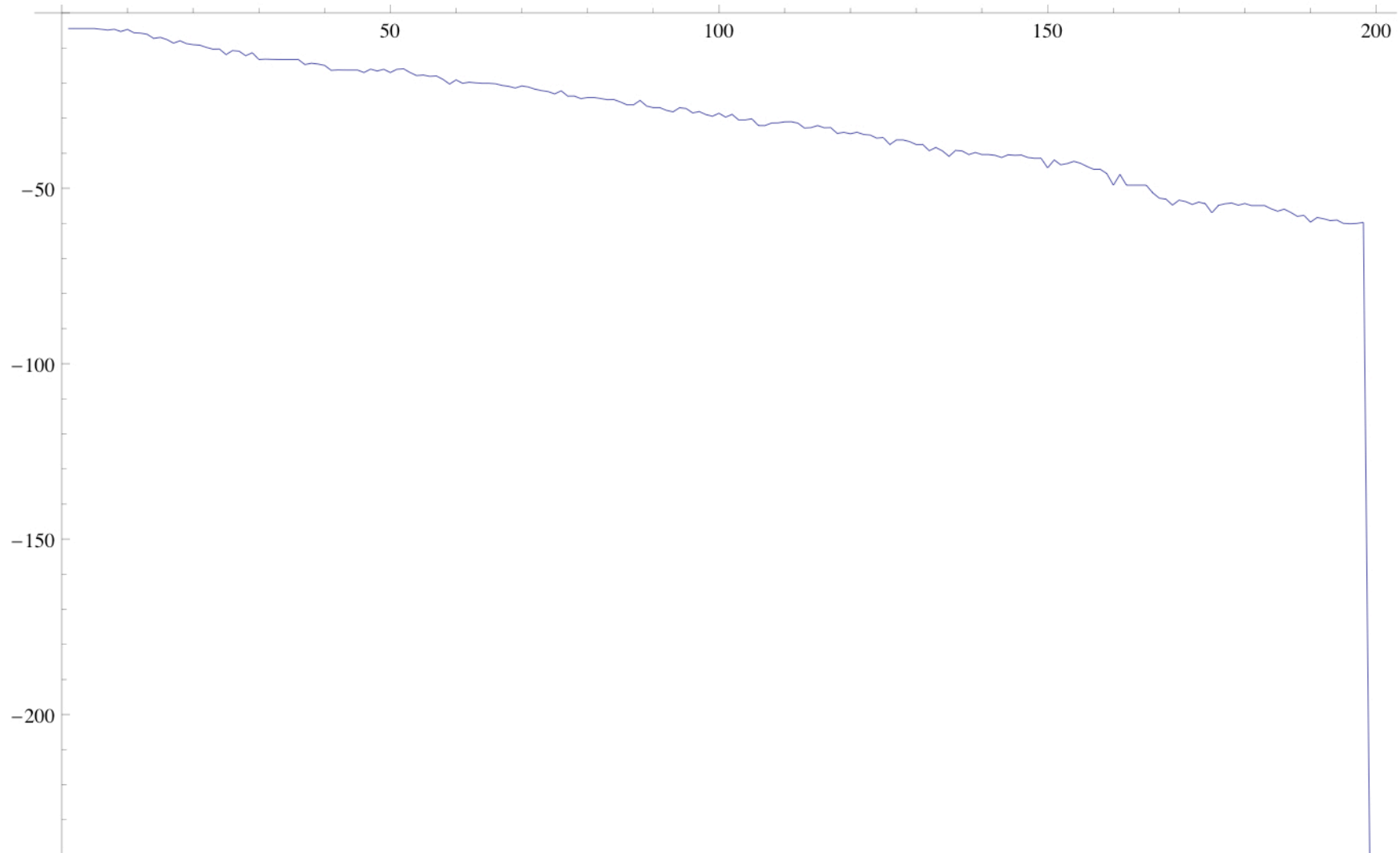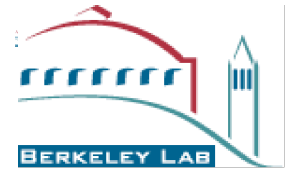
Bifurcation Points in Chaos Theory

Let $t = B_3$ = the smallest r such that the "logistic iteration"

$$x_{n+1} = rx_n(1 - x_n)$$

exhibits 8-way periodicity instead of 4-way periodicity.

By means of a sequential approximation scheme, one can obtain the numerical value of t to any desired precision:

3.5440903595519228536159659866048045405830998454445736754581…

Applying PSLQ to $(1, t, t^2, t^3, …, t^{12})$, we obtained the result that t is a root of the polynomial:

$$0 = 4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7$$
$$-193t^8 - 40t^9 + 48t^{10} - 12t^{11} + t^{12}$$
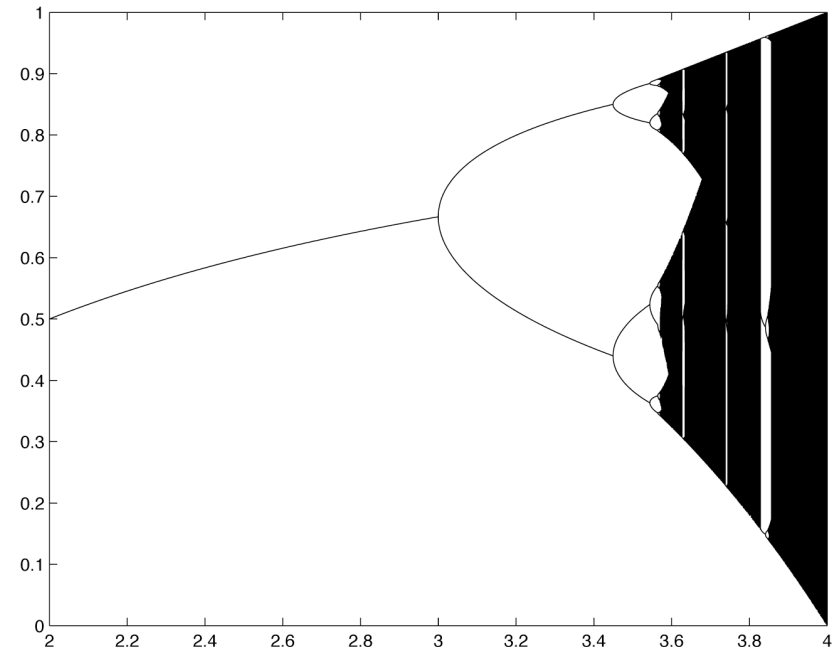
The BBP Formula for Pi

In 1996, at the suggestion of Peter Borwein, Simon Plouffe used DHB's PSLQ program and arbitrary precision software to discover this new formula for π:

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

This formula permits one to compute binary (or hexadecimal) digits of pi beginning at an arbitrary starting position, using a very simple scheme that can run on any system with standard 64-bit or 128-bit arithmetic.

Recently it was proven that no base-n formulas of this type exist for π, except $n = 2^m$.

1. DHB, 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.

2. 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.

Tanh-Sinh Quadrature

Given $f(x)$ defined on (-1,1), define $g(t) = \tanh(\pi/2 \sinh t)$. Then setting $x = g(t)$ yields

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

where $x_j = g(hj)$ and $w_j = g'(hj)$. Since $g'(t)$ goes to zero very rapidly for large t, the product $f(g(t))\,g'(t)$ typically is a nice bell-shaped function for which the Euler-Maclaurin formula implies that the simple summation above is remarkably accurate. Reducing h by half typically doubles the number of correct digits.

For our applications, we have found that tanh-sinh is the best general-purpose integration scheme for functions with vertical derivatives or singularities at endpoints, or for any function at very high precision (> 1000 digits). Otherwise we use Gaussian quadrature.

1. DHB, Xiaoye S. Li and Karthik Jeyabalan, "A Comparison of Three High-Precision Quadrature Schemes," *Experimental Mathematics*, vol. 14 (2005), no. 3, pg. 317-329.
2. H. Takahasi and M. Mori, "Double Exponential Formulas for Numerical Integration," Publications of RIMS, Kyoto University, vol. 9 (1974), pg. 721–741.

Computing High-Precision Values of Multi-Dimension Integrals

Computing multi-hundred digit numerical values of 2-D, 3-D and higher-dimensional integrals remains a major challenge.

Typical approach:

♦ Consider the 2-D or 3-D domain divided into 1-D lines.

♦ Use Gaussian quadrature (for regular functions) or tanh-sinh quadrature (if function has vertical derivates or singularities on boundaries) on each of the 1-D lines.

♦ Discontinue evaluation beyond points where it is clear that function-weight products are smaller than the "epsilon" of the precision level (this works better with tanh-sinh).

Even with "smart" evaluation that avoids unnecessary evaluations, the computational cost increases very sharply with dimension:

♦ If 1000 evaluation points are required in 1-D for a given precision, then typically 1,000,000 are required in 2-D and 1,000,000,000 in 3-D, etc.

The Sparse Grid Scheme

The "sparse grid" scheme for numerical integration in multiple dimensions approximates an integral by evaluating a succession of nested lower-resolution quadrature rules. For example, in two dimensions:
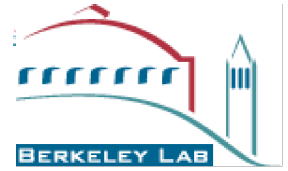
- Level 1: 1x1 (i.e., evaluate function only at origin)
- Level 2: (1x3 + 3x1) – (1x1)
- Level 3: (1x5 + 3x3 + 5x1) – (1x3 + 3x1)
- Level 4: (1x9 + 3x5 + 5x3 + 9x1) – (1x5 + 3x3 + 5x1)
- Level 5: (1x17 + 3x9 + 5x5 + 9x3 + 17x1) – (1x9 + 3x5 + 5x3 + 9x1)

The sparse grid theory shows that for broad classes of functions, this multi-level scheme achieves reasonably fast convergence.

Note that in high dimensions, most points are a relatively far distance from the origin, where the multi-dimensional weight of the quadrature scheme (and, most likely, the function itself) have small values.

Thus a nested scheme (like sparse grid) that avoids the distant "corners" achieves a significant savings in high dimensions.

A Log-Tan Integral Identity

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log\left|\frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}}\right| \, dt \;\; = \;\; L_{-7}(2) \;\; =$$

$$\sum_{n=0}^{\infty} \left[\frac{1}{(7n+1)^2} + \frac{1}{(7n+2)^2} - \frac{1}{(7n+3)^2} + \frac{1}{(7n+4)^2} - \frac{1}{(7n+5)^2} - \frac{1}{(7n+6)^2}\right]$$

This identity arises from analysis of volumes of knot complements in hyperbolic space. This is simplest of 998 related identities.

We have verified this numerically to 20,000 digits (using highly parallel tanh-sinh quadrature).
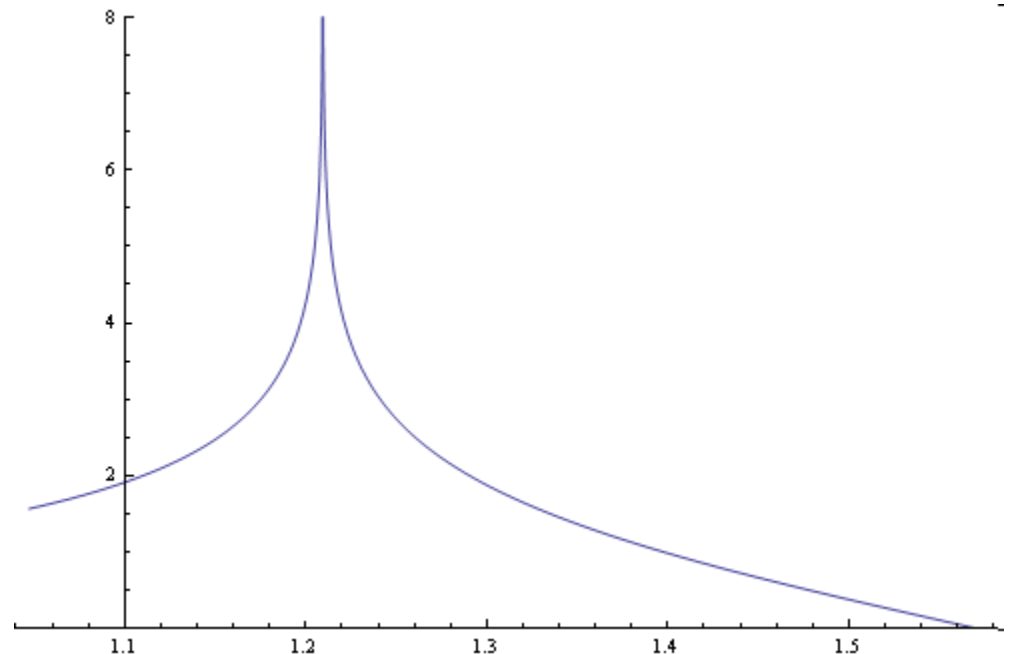
We recently applied our methods to study three classes of integrals that arise in the Ising theory of mathematical physics – D_n and two others:

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

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

$$E_n = 2 \int_0^1 \cdots \int_0^1 \left(\prod_{1 \le j < k \le n} \frac{u_k - u_j}{u_k + u_j}\right)^2 dt_2 \, dt_3 \cdots dt_n$$

where in the last line $u_k = t_1 t_2 \ldots t_k$.

DHB, J. M. Borwein and R. E. Crandall, "Integrals of the Ising Class," *Journal of Physics A: Mathematical and General*, vol. 39 (2006), pg. 12271-12302.

We observed that the multi-dimensional C_n integrals can be transformed to 1-D integrals:

$$C_n \;=\; \frac{2^n}{n!} \int_0^\infty t K_0^n(t) \, \mathrm{d}t$$

where K_0 is the modified Bessel function. In this form, the C_n constants appear naturally in in quantum field theory (QFT).

We used this formula to compute 1000-digit numerical values of various C_n, from which the following results and others were found, then proven:

$$C_1 \;=\; 2$$

$$C_2 \;=\; 1$$

$$C_3 \;=\; \mathrm{L}_{-3}(2) \;=\; \sum_{n \geq 0} \left(\frac{1}{(3n+1)^2} - \frac{1}{(3n+2)^2} \right)$$

$$C_4 \;=\; \frac{7}{12} \zeta(3)$$

The C_n numerical values appear to approach a limit. For instance,

$$C_{1024} = 0.6304735033743867961220401927108789043545870787127 3234\ldots$$

What is this limit? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator (ISC):

http://ddrive.cs.dal.ca/~isc

The result was:

$$\lim_{n \to \infty} C_n = 2e^{-2\gamma}$$

where gamma denotes Euler's constant. Finding this limit led us to the asymptotic expansion and made it clear that the integral representation of C_n is fundamental.

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$$D_2 = 1/3$$

$$D_3 = 8 + 4\pi^2/3 - 27\,\mathrm{L}_{-3}(2)$$

$$D_4 = 4\pi^2/9 - 1/6 - 7\zeta(3)/2$$

$$E_2 = 6 - 8\log 2$$

$$E_3 = 10 - 2\pi^2 - 8\log 2 + 32\log^2 2$$

$$E_4 = 22 - 82\zeta(3) - 24\log 2 + 176\log^2 2 - 256(\log^3 2)/3$$
$$+ 16\pi^2\log 2 - 22\pi^2/3$$

$$E_5 \stackrel{?}{=} 42 - 1984\,\mathrm{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3)\log 2$$
$$+ 40\pi^2\log^2 2 - 62\pi^2/3 + 40(\pi^2\log 2)/3 + 88\log^4 2$$
$$+ 464\log^2 2 - 40\log 2$$

where $\mathrm{Li}_n(x)$ is the polylog function. D_2, D_3 and D_4 were originally provided to us by mathematical physicist Craig Tracy, who hoped that our tools could help identify D_5.

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

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

We also computed D_5 to 500 digits, but were unable to identify it. The digits are available if anyone wishes to further explore this question.

$$E_5 = \int_0^1 \int_0^1 \int_0^1 \left[2(1-x)^2(1-y)^2(1-xy)^2(1-z)^2(1-yz)^2(1-xyz)^2 \right.$$

$$\left(- \left[4(x+1)(xy+1)\log(2)\left(y^5 z^3 x^7 - y^4 z^2 (4(y+1)z+3)x^6 - y^3 z \left((y^2+1)z^2 + 4(y+1)z+5 \right) x^5 + y^2 \left(4y(y+1)z^3 + 3(y^2+1)z^2 + 4(y+1)z-1 \right) x^4 + y \left(z \left(z^2 + 4z +5 \right) y^2 + 4(z^2+1)y + 5z + 4 \right) x^3 + \left((-3z^2-4z+1)y^2 - 4zy + 1 \right) x^2 - (y(5z+4)+4)x - 1 \right) \right] / \left[(x-1)^3 (xy-1)^3 (xyz-1)^3 \right] + \left[3(y-1)^2 y^4 (z-1)^2 z^2 (yz-1)^2 x^6 + 2y^3 z \left(3(z-1)^2 z^3 y^5 + z^2 \left(5z^3 + 3z^2 + 3z + 5 \right) y^4 + (z-1)^2 z \left(5z^2 + 16z + 5 \right) y^3 + \left(3z^5 + 3z^4 - 22z^3 - 22z^2 + 3z + 3 \right) y^2 + 3 \left(-2z^4 + z^3 + 2z^2 + z - 2 \right) y + 3z^3 + 5z^2 + 5z + 3 \right) x^5 + y^2 \left(7(z-1)^2 z^4 y^6 - 2z^3 \left(z^3 + 15z^2 + 15z + 1 \right) y^5 + 2z^2 \left(-21z^4 + 6z^3 + 14z^2 + 6z - 21 \right) y^4 - 2z \left(z^5 - 6z^4 - 27z^3 - 27z^2 - 6z + 1 \right) y^3 + \left(7z^6 - 30z^5 + 28z^4 + 54z^3 + 28z^2 - 30z + 7 \right) y^2 - 2 \left(7z^5 + 15z^4 - 6z^3 - 6z^2 + 15z + 7 \right) y + 7z^4 - 2z^3 - 42z^2 - 2z + 7 \right) x^4 - 2y \left(z^3 \left(z^3 - 9z^2 - 9z + 1 \right) y^6 + z^2 \left(7z^4 - 14z^3 - 18z^2 - 14z + 7 \right) y^5 + z \left(7z^5 + 14z^4 + 3z^3 + 3z^2 + 14z + 7 \right) y^4 + \left(z^6 - 14z^5 + 3z^4 + 84z^3 + 3z^2 - 14z + 1 \right) y^3 - 3 \left(3z^5 + 6z^4 - z^3 - z^2 + 6z + 3 \right) y^2 - \left(9z^4 + 14z^3 - 14z^2 + 14z + 9 \right) y + z^3 + 7z^2 + 7z + 1 \right) x^3 + \left(z^2 \left(11z^4 + 6z^3 - 66z^2 + 6z + 11 \right) y^6 + 2z \left(5z^5 + 13z^4 - 2z^3 - 2z^2 + 13z + 5 \right) y^5 + \left(11z^6 + 26z^5 + 44z^4 - 66z^3 + 44z^2 + 26z + 11 \right) y^4 + \left(6z^5 - 4z^4 - 66z^3 - 66z^2 - 4z + 6 \right) y^3 - 2 \left(33z^4 + 2z^3 - 22z^2 + 2z + 33 \right) y^2 + \left(6z^3 + 26z^2 + 26z + 6 \right) y + 11z^2 + 10z + 11 \right) x^2 - 2 \left(z^2 \left(5z^3 + 3z^2 + 3z + 5 \right) y^5 + z \left(22z^4 + 5z^3 - 22z^2 + 5z + 22 \right) y^4 + \left(5z^5 + 5z^4 - 26z^3 - 26z^2 + 5z + 5 \right) y^3 + \left(3z^4 - 22z^3 - 26z^2 - 22z + 3 \right) y^2 + \left(3z^3 + 5z^2 + 5z + 3 \right) y + 5z^2 + 22z + 5 \right) x + 15z^2 + 2z + 2y(z-1)^2(z+1) + 2y^3(z-1)^2 z(z+1) + y^4 z^2 \left(15z^2 + 2z + 15 \right) + y^2 \left(15z^4 - 2z^3 - 90z^2 - 2z + 15 \right) + 15 \right] / \left[(x-1)^2 (y-1)^2 (xy-1)^2 (z-1)^2 (yz-1)^2 (xyz-1)^2 \right] - \left[4(x+1)(y+1)(yz+1) \left(-z^2 y^4 + 4z(z+1)y^3 + (z^2+1)y^2 - 4(z+1)y + 4x \left(y^2 - 1 \right) \left(y^2 z^2 - 1 \right) + x^2 \left(z^2 y^4 - 4z(z+1)y^3 - (z^2+1)y^2 + 4(z+1)y + 1 \right) - 1 \right) \log(x+1) \right] / \left[(x-1)^3 x(y-1)^3 (yz-1)^3 \right] - \left[4(y+1)(xy+1)(z+1) \left(x^2 \left(z^2 - 4z - 1 \right) y^4 + 4x(x+1) \left(z^2 - 1 \right) y^3 - \left(x^2 + 1 \right) \left(z^2 - 4z - 1 \right) y^2 - 4(x+1) \left(z^2 - 1 \right) y + z^2 - 4z - 1 \right) \log(xy+1) \right] / \left[x(y-1)^3 y(xy-1)^3 (z-1)^3 \right] - \left[4(z+1)(yz+1) \left(x^3 y^5 z^7 + x^2 y^4 (4x(y+1)+5)z^6 - xy^3 \left((y^2+1)x^2 - 4(y+1)x - 3 \right) z^5 - y^2 \left(4y(y+1)x^3 + 5 \left(y^2 + 1 \right) x^2 + 4(y+1)x + 1 \right) z^4 + y \left(y^2 x^3 - 4y(y+1)x^2 - 3 \left(y^2 + 1 \right) x - 4(y+1) \right) z^3 + \left(5x^2 y^2 + y^2 + 4x(y+1)y + 1 \right) z^2 + ((3x+4)y+4)z - 1 \right) \log(xyz+1) \right] / \left[xy(z-1)^3 z(yz-1)^3 (xyz-1)^3 \right] \right) / \left[(x+1)^2 (y+1)^2 (xy+1)^2 (z+1)^2 (yz+1)^2 (xyz+1)^2 \right] \, dx \, dy \, dz$$
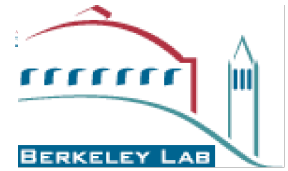
Consider the 2-parameter class of Ising integrals (which arises in QFT for odd k):

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

After computing 1000-digit numerical values for all n up to 36 and all k up to 75 (performed on a highly parallel computer system), we discovered (using PSLQ) linear relations in the rows of this array. For example, when $n = 3$:

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

Similar, but more complicated, recursions have been found for all n.

DHB, D. Borwein, J. M. Borwein and R. Crandall, "Hypergeometric Forms for Ising-Class Integrals," *Experimental Mathematics*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/meijer/pdf.

J. M. Borwein and B. Salvy, "A Proof of a Recursion for Bessel Moments," *Experimental Mathematics*, vol. 17 (2008), pg. 223-230.

$$c_{3,0} = \frac{3\Gamma^6(1/3)}{32\pi 2^{2/3}} = \frac{\sqrt{3}\pi^3}{8}\, {}_3F_2\left(\begin{array}{c} 1/2, 1/2, 1/2 \\ 1, 1 \end{array}\middle|\, \frac{1}{4}\right)$$

$$c_{3,2} = \frac{\sqrt{3}\pi^3}{288}\, {}_3F_2\left(\begin{array}{c} 1/2, 1/2, 1/2 \\ 2, 2 \end{array}\middle|\, \frac{1}{4}\right)$$

$$c_{4,0} = \frac{\pi^4}{4}\sum_{n=0}^{\infty}\frac{\binom{2n}{n}^4}{4^{4n}} = \frac{\pi^4}{4}\, {}_4F_3\left(\begin{array}{c} 1/2, 1/2, 1/2, 1/2 \\ 1, 1, 1 \end{array}\middle|\, 1\right)$$

$$c_{4,2} = \frac{\pi^4}{64}\left[4\, {}_4F_3\left(\begin{array}{c} 1/2, 1/2, 1/2, 1/2 \\ 1, 1, 1 \end{array}\middle|\, 1\right)\right.$$
$$\left. -3\, {}_4F_3\left(\begin{array}{c} 1/2, 1/2, 1/2, 1/2 \\ 2, 1, 1 \end{array}\middle|\, 1\right)\right] - \frac{3\pi^2}{16}$$

2-D Integral in Bessel Moment Study

We conjectured (and later proved)

$$c_{5,0} = \frac{\pi}{2} \int_{-\pi/2}^{\pi/2} \int_{-\pi/2}^{\pi/2} \frac{\mathbf{K}(\sin\theta)\,\mathbf{K}(\sin\phi)}{\sqrt{\cos^2\theta\cos^2\phi + 4\sin^2(\theta+\phi)}}\,\mathrm{d}\theta\,\mathrm{d}\phi$$

Here **K** denotes the complete elliptic integral of the first kind

Note that the integrand function has singularities on all four sides of the region of integration.

We were able to evaluate this integral to 120-digit accuracy, using 1024 cores of the "Franklin" Cray XT4 system at LBNL.
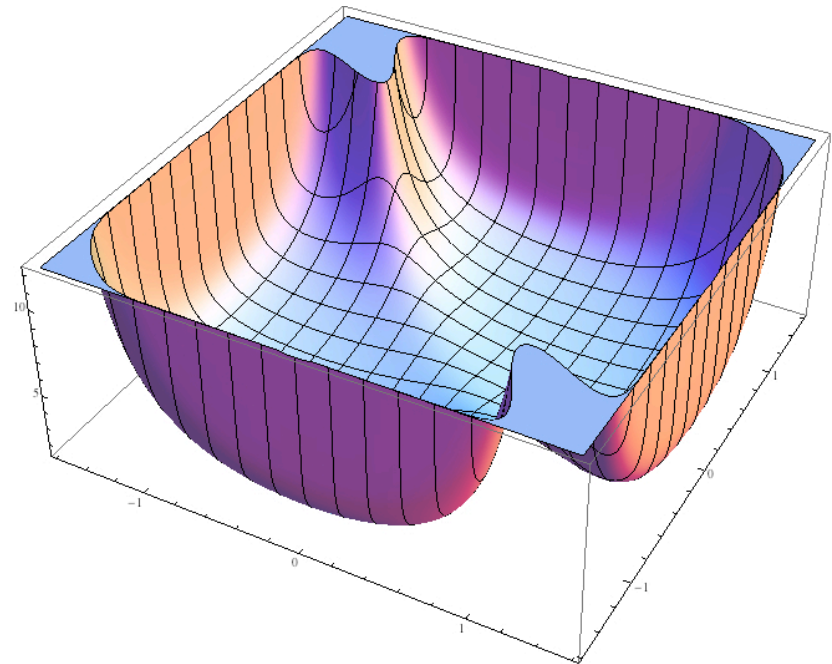
In another recent application of these methods, we investigated the following "spin integrals," which arise from studies in mathematical physics:
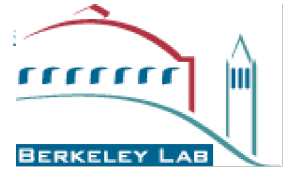
$$P(n) := \frac{\pi^{n(n+1)/2}}{(2\pi i)^n} \cdot \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2)$$
$$\times\, T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2)\, \mathrm{d}x_1 \mathrm{d}x_2 \cdots \mathrm{d}x_n$$

where

$$U(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) = \frac{\prod_{1 \le k < j \le n} \sinh[\pi(x_j - x_k)]}{\prod_{1 \le j \le n} i^n \cosh^n(\pi x_j)}$$

$$T(x_1 - i/2, x_2 - i/2, \cdots, x_n - i/2) = \frac{\prod_{1 \le j \le n}(x_j - i/2)^{j-1}(x_j + i/2)^{n-j}}{\prod_{1 \le k < j \le n}(x_j - x_k - i)}$$

H. E. Boos, V. E. Korepin, Y. Nishiyama and M. Shiroishi, "Quantum Correlations and Number Theory," *Journal of Physics A: Mathematical and General*, vol. 35 (2002), pg. 4443.

Evaluations of *P(n)*
Derived Analytically, Confirmed Numerically

$$P(1) = \frac{1}{2}, \quad P(2) = \frac{1}{3} - \frac{1}{3}\log 2, \quad P(3) = \frac{1}{4} - \log 2 + \frac{3}{8}\zeta(3)$$

$$P(4) = \frac{1}{5} - 2\log 2 + \frac{173}{60}\zeta(3) - \frac{11}{6}\zeta(3)\log 2 - \frac{51}{80}\zeta^2(3) - \frac{55}{24}\zeta(5) + \frac{85}{24}\zeta(5)\log 2$$

$$P(5) = \frac{1}{6} - \frac{10}{3}\log 2 + \frac{281}{24}\zeta(3) - \frac{45}{2}\zeta(3)\log 2 - \frac{489}{16}\zeta^2(3) - \frac{6775}{192}\zeta(5)$$

$$+ \frac{1225}{6}\zeta(5)\log 2 - \frac{425}{64}\zeta(3)\zeta(5) - \frac{12125}{256}\zeta^2(5) + \frac{6223}{256}\zeta(7)$$

$$- \frac{11515}{64}\zeta(7)\log 2 + \frac{42777}{512}\zeta(3)\zeta(7)$$

and a much more complicated expression for *P*(6). Run times increase very rapidly with the dimension *n*:

n	Digits	Processors	Run Time
2	120	1	10 sec.
3	120	8	55 min.
4	60	64	27 min.
5	30	256	39 min.
6	6	256	59 hrs.

The following integrals appear in studies, say, of the average distance between points in a cube, or the average electric potential in a cube:

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

$$\Delta_n(s) := \int_0^1 \cdots \int_0^1 \left((r_1 - q_1)^2 + \cdots + (r_n - q_n)^2 \right)^{s/2} \, dr_1 \cdots dr_n \, dq_1 \cdots dq_n$$

DHB, J. M. Borwein and R. E. Crandall, "Box Integrals," *Journal of Computational and Applied Mathematics*, vol. 206 (2007), pg. 196-208.

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

$$B_3(-1) = -\frac{\pi}{4} - \frac{1}{2}\log 2 + \log(5 + 3\sqrt{3})$$

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

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

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

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

where

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

$$\Delta_2(-1) = \frac{4}{3} - \frac{4}{3}\sqrt{2} + 4\log(1 + \sqrt{2})$$

$$\Delta_1(1) = \frac{1}{3}$$

$$\Delta_2(1) = \frac{1}{15}\left(2 + \sqrt{2} + 5\log(1 + \sqrt{2})\right),$$

$$\Delta_3(1) = \frac{4}{105} + \frac{17}{105}\sqrt{2} - \frac{2}{35}\sqrt{3} + \frac{1}{5}\log(1 + \sqrt{2}) + \frac{2}{5}\log(2 + \sqrt{3}) - \frac{1}{15}\pi,$$

$$\Delta_4(1) = \frac{26}{15}G - \frac{34}{105}\pi\sqrt{2} - \frac{16}{315}\pi + \frac{197}{420}\log(3) + \frac{52}{105}\log\left(2 + \sqrt{3}\right)$$

$$+ \frac{1}{14}\log\left(1 + \sqrt{2}\right) + \frac{8}{105}\sqrt{3} + \frac{73}{630}\sqrt{2} - \frac{23}{135} + \frac{136}{105}\sqrt{2}\arctan\left(\frac{1}{\sqrt{2}}\right)$$

$$- \frac{1}{5}\pi\log\left(1 + \sqrt{2}\right) + \frac{4}{5}\alpha\log\left(1 + \sqrt{2}\right) - \frac{4}{5}\mathrm{Cl}_2(\alpha) - \frac{4}{5}\mathrm{Cl}_2\left(\alpha + \frac{\pi}{2}\right)$$

where G is Catalan's constant and Cl denotes the Clausen function.

$$\Delta_3(-1) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{(-1 + e^{-u^2} + \sqrt{\pi}\, u\, \mathrm{erf}(u))^3}{u^6}\, \mathrm{d}u$$

$$= \frac{1}{15}\left(6 + 6\sqrt{2} - 12\sqrt{3} - 10\pi + 30\log(1 + \sqrt{2}) + 30\log(2 + \sqrt{3})\right)$$

As in many of the previous results, this was found by first computing the integral to high precision (250 to 1000 digits), conjecturing possible terms on the right-hand side, then applying PSLQ to look for a relation. We now have proven this result.

This and similar integrals have recently arisen in problems suggested by neuroscientists – e.g., the average distance between synapses in a mouse brain.

Ref: Work in progress! Will be written up soon.

Summary

- Numerous state-of-the-art large-scale scientific calculations now require numerical precision beyond conventional 64-bit floating-point arithmetic.

- The emerging "experimental" methodology in mathematics and mathematical physics often requires hundreds or even thousands of digits of precision.

- Double-double, quad-double and arbitrary precision software libraries are now widely available (and in most cases are free).

- High-precision evaluation of integrals, followed by constant-recognition techniques, has been a particularly fruitful area of recent research, with many new results in mathematics and mathematical physics.

- There is a critical need to develop faster techniques for high-precision numerical integration in multiple dimensions.