Peter Borwein and High-Performance Computing

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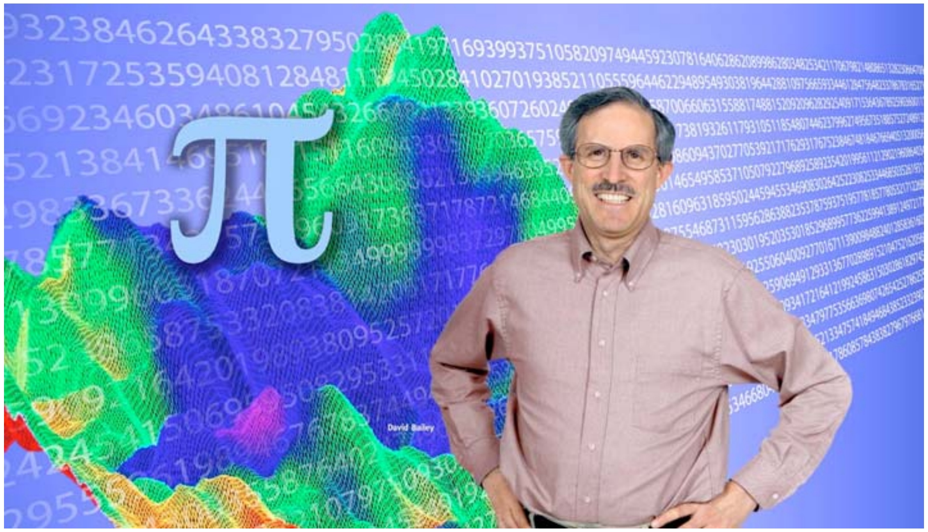
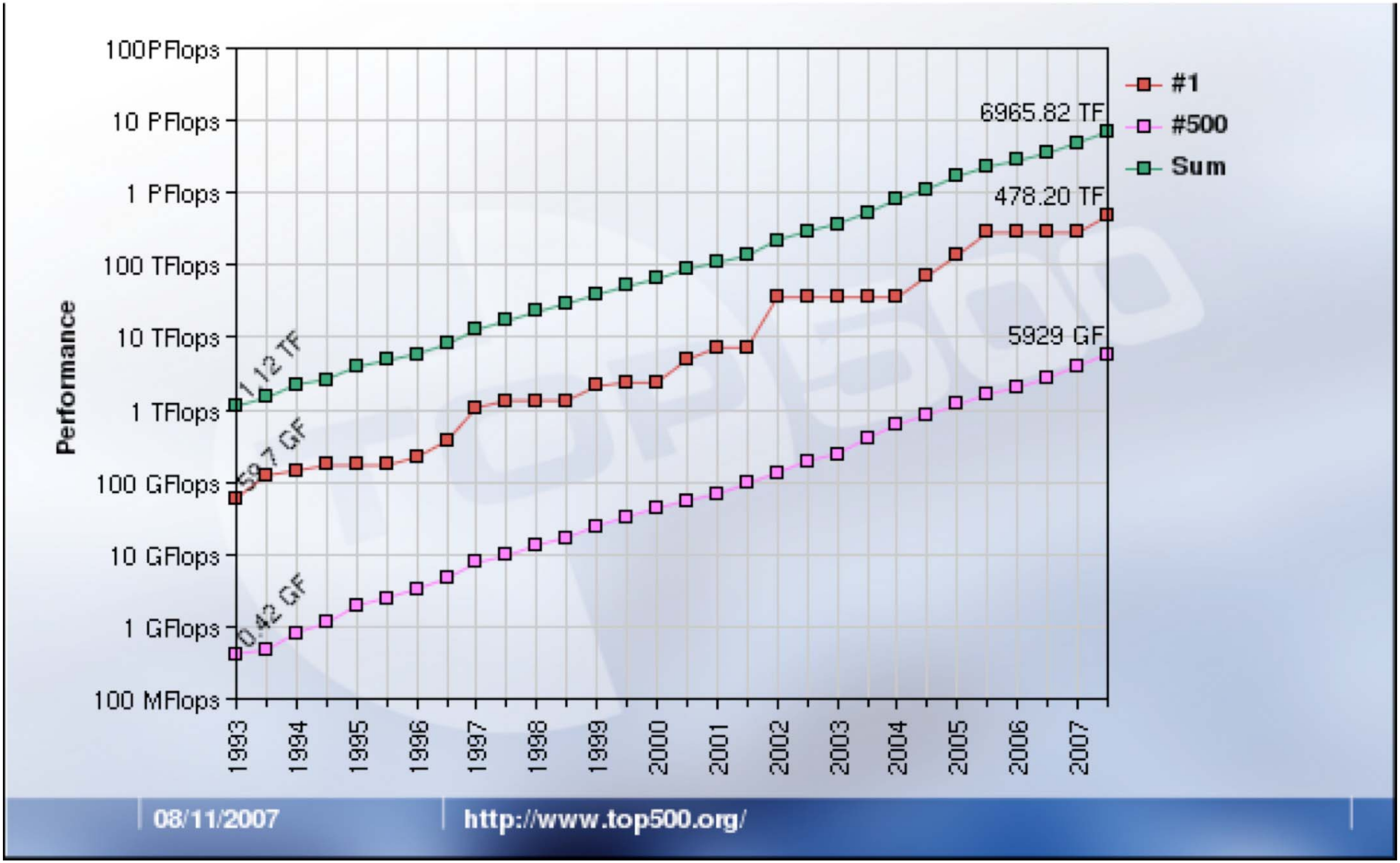
This talk is available at:
`http://crd.lbl.gov/~dhbailey/dhbtalks/dhb-peter-borwein.pdf`



Experimental Mathematics: The Application of High-Performance Computing to Mathematical Research

- An experimental approach ties mathematical research to Moore's Law, which has been advancing at an exponential rate for over 40 years.
- Additional advances have resulted from improved algorithms, numerical techniques and progamming methodology.
- Experimental mathematics is a delightfully multidisciplinary activity -- pure mathematicians, applied mathematicians, computer scientists, numerical analysts and physicists have all made notable contributions.
- Experimental mathematics is a delightfully non-hierarchical activity -- even undergraduate students, armed with good programming skills, can obtain significant research results.

Top500 Performance Trends

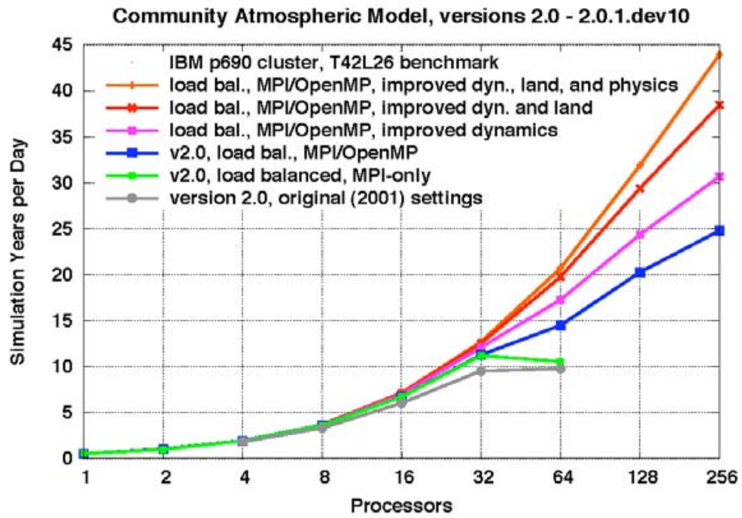


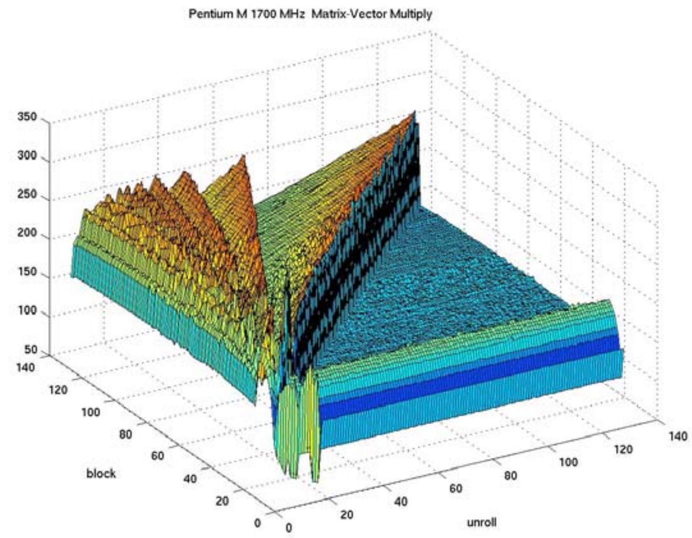
The "Franklin" System at LBNL's NERSC Computer Center

- 9,660 dual-core Opteron computational nodes (19,320 CPUs).
- 100 Tflop/s (100 trillion floating-point operations / sec) peak performance.
- 38.6 Tbytes (38.6 trillion bytes) main memory.

The SciDAC Performance Engineering Research Institute (PERI)

- Participating institutions: Argonne, LBNL, LLNL, Oak Ridge, Rice, UCSD, U Maryland, UNC, USC, U Tennessee.
- Lead investigators: Robert Lucas, USC/ISI and David H Bailey, LBNL.
- Funding: $4 million per year.
- Mission: To improve the performance of DOE-funded science applications on high-end computing platforms.
- Component activities:
  - Performance modeling.
  - Automatic performance tuning.
  - Application engagement.





Key Ideas in My Research and Their Roots in Peter Borwein's Work

- Employing custom variations of FFTs to accelerate computations on new vector and parallel computer architectures.
  - This dates back to 1985, when I used Jon and Peter's quartic algorithm to compute pi to millions of decimal digits on a new Cray-2 supercomputer.
- Employing Ferguson's "PSLQ" algorithm to discover new mathematical identities, based on high-precision numerical values of constants.
  - The first instance was in 1996, when Peter, Simon Plouffe and myself used a PSLQ program to discover the BBP formula for pi.
- Proving that certain classes of explicit constants are "normal" (i.e., that the digit sequence is "random" in a certain specific sense).
  - This work, done with Richard Crandall, had its roots in the BBP formula.
- Computing high-precision values of multi-zeta constants and identifying them in terms of more basic constants.
  - I utilized Peter's formula for zeta(n) to compute high-precision values.
- Using the tanh-sinh and other Euler-Macluarin based schemes to compute definite integrals to very high precision.
  - This had its roots about 12 years ago when working on a problem of Peter Borwein to numerically integrate functions of the form f(t) exp(-t^2/2).

High-Precision Computation

Most scientific computation utilizes floating-point arithmetic (although some, such genome sequence analysis, use only integer computations).

Present-day computer hardware supports three types of floating-point:

- IEEE 32-bit (“single precision”), roughly 6 digits.
- IEEE 64-bit (“double precision”), roughly 16 digits.
- IEEE 80-bit (“extended precision”), roughly 18 digits (Intel and AMD).

For a growing number of computations, much higher precision is needed:

- Quantum field theory.
- Supernova simulation.
- Semiconductor physics.
- Planetary orbit calculations.
- Ising theory of mathematical physics.
- Experimental and computational mathematics.

Using FFTs to Accelerate High-Precision Arithmetic

- Let A and B be high-precision numerical values represented as n-long strings of computer words, where each word contain b bits of precision.
- Note that C = A x B is merely the convolution of A and B, where A and B are first extended to length 2n by padding with zeros:
  - $C_k = \text{Sum } A_j \, B_{k-j}$
- This requires 2 n^2 individual arithmetic operations. But convolutions can be performed rapidly using FFTs:
  - $C = FFT^{-1} \, [FFT(A) \;\; FFT(B)]$
- If this is done efficiently, the operation count is reduced to 15 $n \log_2 n$ operations, which is fewer than the standard count when n > 16.
- In real-world computations, when all the software overhead is taken into account, FFT-based arithmetic is faster for computations of 1000+ digits.
- Other operations, including division and square roots, can be performed via Newton iterations, based on FFT-accelerated multiplication.
- Algorithms of Richard Brent and Peter and Jon Borwein can be used to compute high-precision exp and trig functions, and constants such as pi.

LBNL’s High-Precision Software: ARPREC and QD

- QD: Double-double (32 digits) and quad-double (64 digits) .
- ARPREC: Arbitrary precision (hundreds or thousands of digits).
- Low-level routines written in C++.
- High-level C++ and F-90 translation modules permit use with existing programs with only minor code changes.
- Integer, real and complex datatypes.
- Many common functions: sqrt, cos, exp, gamma, etc.
- PSLQ, root finding, numerical integration.
- An interactive “Experimental Mathematician’s Toolkit.”
- Can easily be incorporated into a highly parallel program.

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

Other widely used high-precision software:

- GMP: `http://gmplib.org`
- MPFR: `http://www.mpfr.org`

D. H. Bailey, Y. Hida, X. S. Li and B. Thompson, "ARPREC: An Arbitrary Precision Computation Package," manuscript, Sept 2002, http://crd.lbl.gov/~dhbailey/dhbpapers/arprec.pdf.

The PSLQ Integer Relation Algorithm: A Tool to Discover Mathematical Relationships

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

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

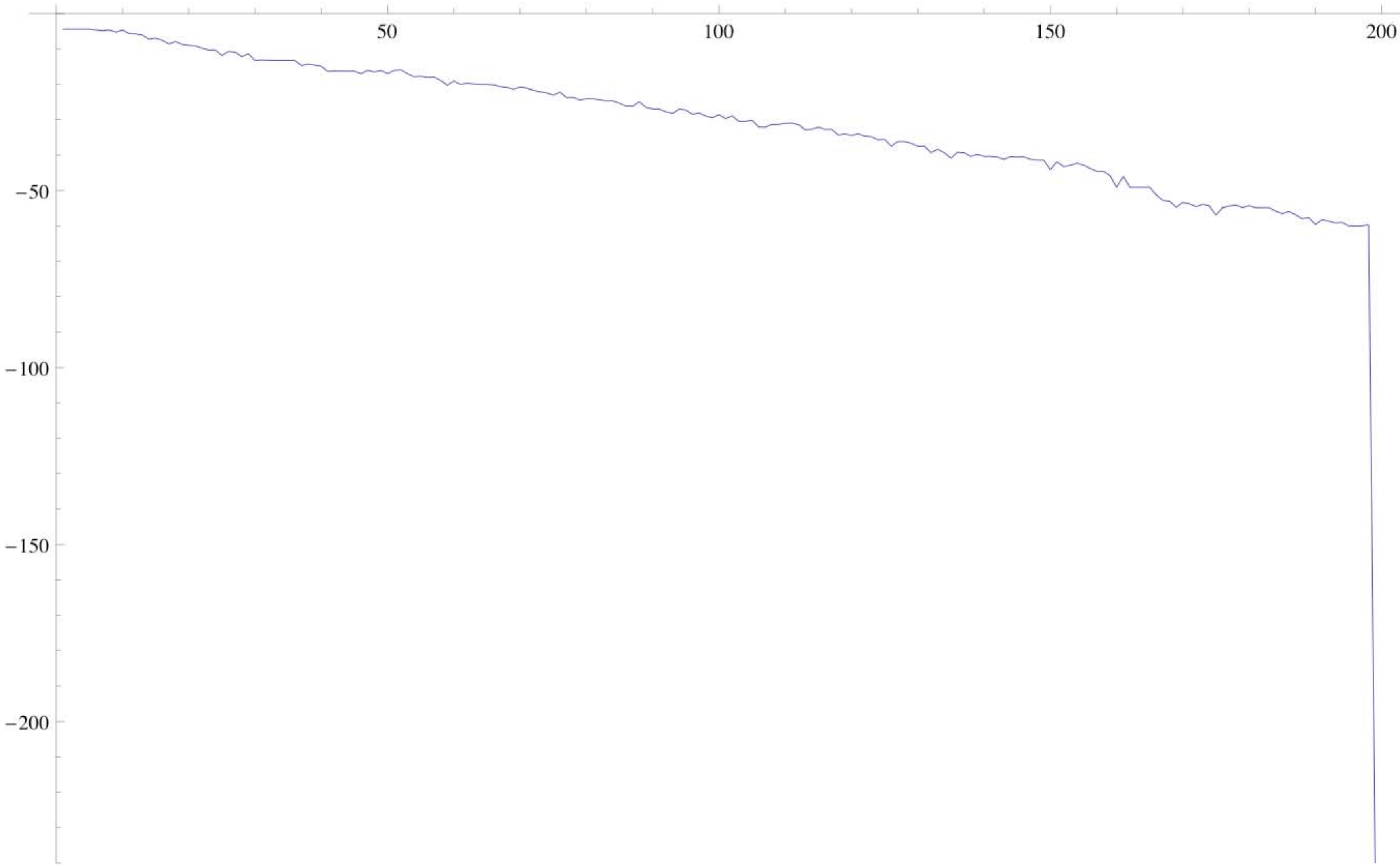
(or within "epsilon" of zero, where epsilon = 10^{-p} and p is the precision).

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, 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.

Decrease of $\log_{10}(\min |x_i|)$ in PSLQ

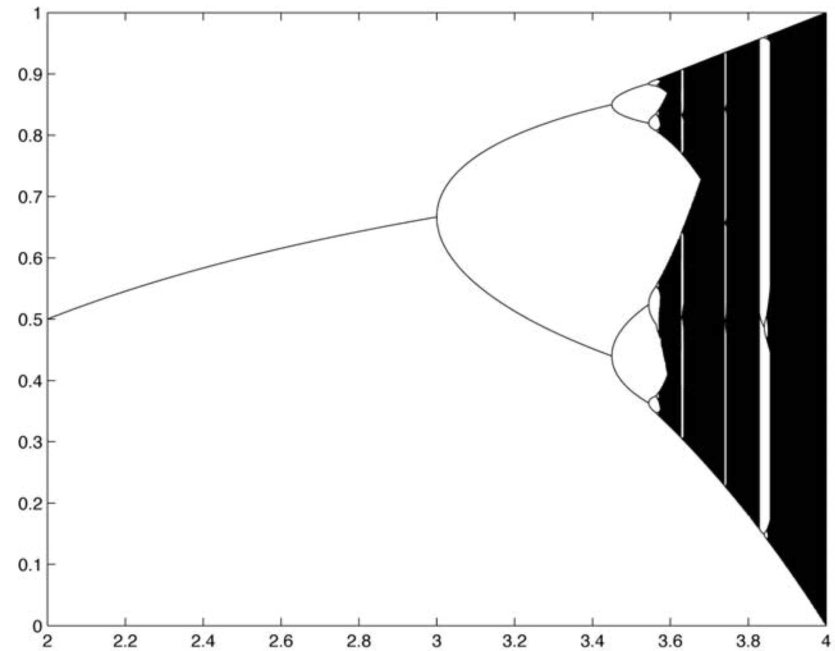


Application of PSLQ: Bifurcation Points in Chaos Theory

Let t be the smallest r such that the "logistic iteration"

$$x_{n+1} \;=\; r x_n (1 - x_n)$$

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



By means of an iterative scheme, one can obtain the numerical value of t to any desired precision:

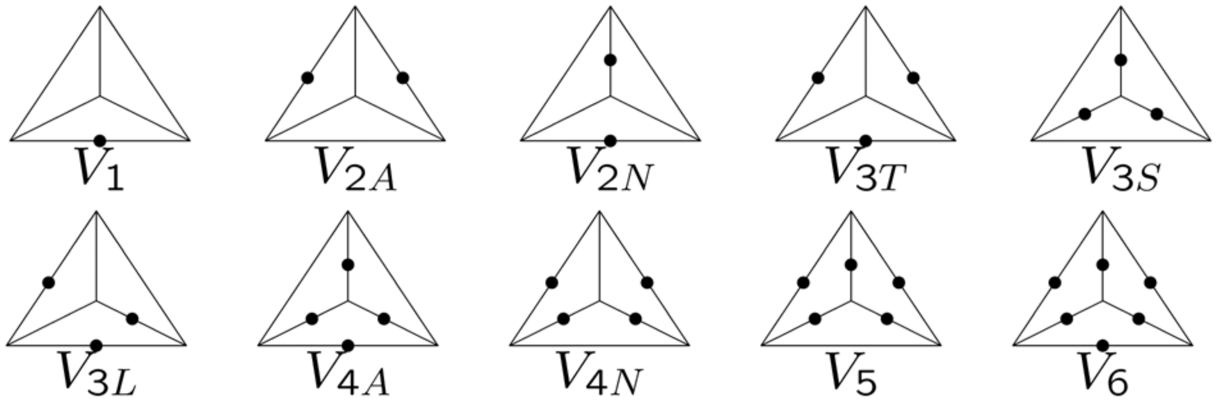
3.544090359551922853615965986604804540583099845444573675457815...

Applying PSLQ to the vector $(1, t, t^2, t^3, \ldots, t^{12})$, one finds that t satisfies:

$$\begin{aligned} 0 \;=\; & 4913 + 2108t^2 - 604t^3 - 977t^4 + 8t^5 + 44t^6 + 392t^7 \\ & -193t^8 - 40t^9 + 48t^{10} - 12t^{11} + t^{12} \end{aligned}$$

David H. Bailey, Jonathan M. Borwein, Vishal Kapoor and Eric Weisstein, "Ten Problems in Experimental Mathematics," *American Mathematical Monthly*, vol. 113, no. 6 (Jun 2006), pg. 481-409.

Application of PSLQ: Identifying Ten Constants from Quantum Field Theory



$$
\begin{aligned}
V_1 &= 6\zeta(3) + 3\zeta(4) \\
V_{2A} &= 6\zeta(3) - 5\zeta(4) \\
V_{2N} &= 6\zeta(3) - \frac{13}{2}\zeta(4) - 8U \\
V_{3T} &= 6\zeta(3) - 9\zeta(4) \\
V_{3S} &= 6\zeta(3) - \frac{11}{2}\zeta(4) - 4C^2 \\
V_{3L} &= 6\zeta(3) - \frac{15}{4}\zeta(4) - 6C^2 \\
V_{4A} &= 6\zeta(3) - \frac{77}{12}\zeta(4) - 6C^2 \\
V_{4N} &= 6\zeta(3) - 14\zeta(4) - 16U
\end{aligned}
$$

$$
\begin{aligned}
V_5 &= 6\zeta(3) - \frac{469}{27}\zeta(4) + \frac{8}{3}C^2 - 16V \\
V_6 &= 6\zeta(3) - 13\zeta(4) - 8U - 4C^2
\end{aligned}
$$

where

$$
\begin{aligned}
C &= \sum_{k>0} \sin(\pi k/3)/k^2 \\
U &= \sum_{j>k>0} \frac{(-1)^{j+k}}{j^3 k} \\
V &= \sum_{j>k>0} (-1)^j \cos(2\pi k/3)/(j^3 k)
\end{aligned}
$$

Some Supercomputer-Class PSLQ Solutions

- Identification of B_4, the fourth bifurcation point of the logistic iteration:
  Integer relation of size 121. 10,000-digit arithmetic.
- Identification of Apery sums.
  15 integer relation problems, with size up to 118. 5,000-digit arithmetic.
- Identification of Euler-zeta sums.
  Hundreds of integer relation problems, each of size 145. 5,000-digit arithmetic.
- Finding recursions in Ising integrals.
  Over 2600 high-precision numerical integrations, and integer relation detections. 1500-digit arithmetic. Run on Apple system at Virginia Tech – 12 hours on 64 CPUs.
- Finding a relation involving a root of Lehmer's polynomial.
  Integer relation of size 125. 50,000-digit arithmetic. Utilizes 3-level, multi-pair parallel PSLQ program. Run on IBM parallel system – 16 hours on 64 CPUs.

1. 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.
2. D. H. Bailey, D. Borwein, J. M. Borwein and R. Crandall, "Hypergeometric Forms for Ising-Class Integrals," *Experimental Mathematics*, vol. 16 (2007), no. 3, pg. 257-276.

Fascination With Pi

Newton (1670):

"I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

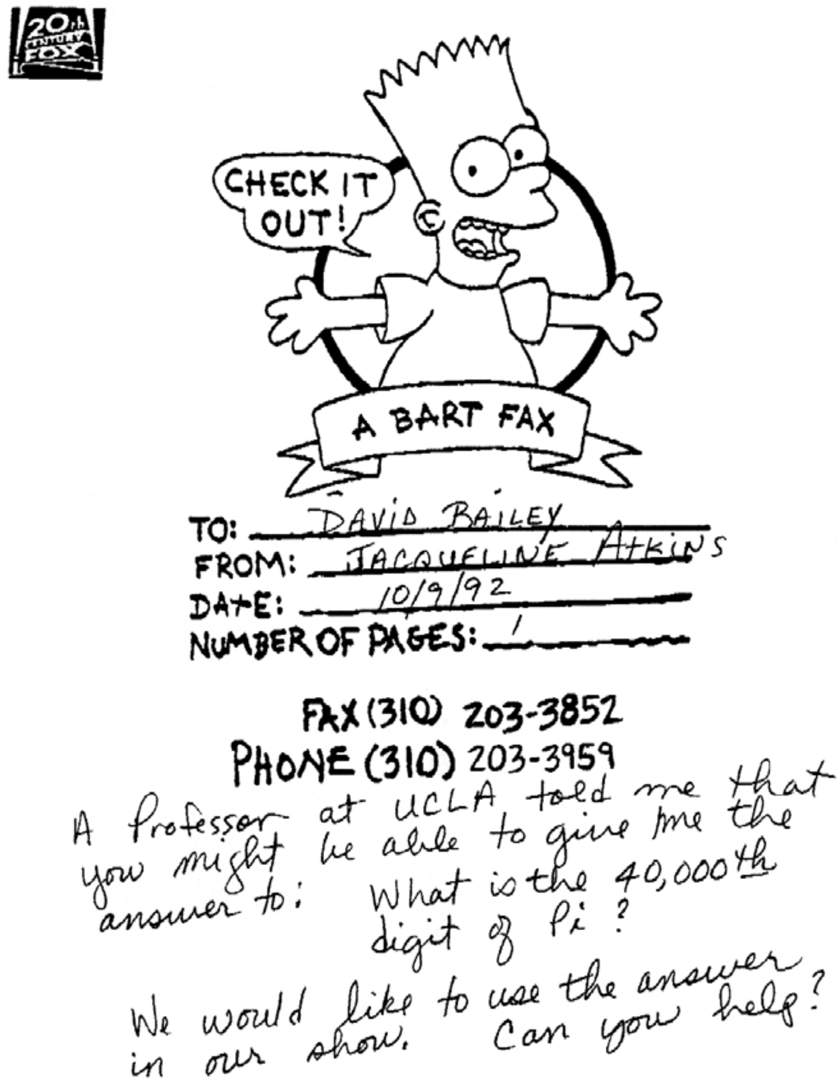
Carl Sagan (1986):

In his book "Contact," the lead scientist (played by Jodie Foster in the movie) looked for patterns in the digits of pi.

New York Times (2007):

On March 14 (03/14) the daily crossword puzzle featured a pi theme: key answers included "pi" in the place of a single character.

Fax from “The Simpsons” Show



TO: DAVID BAILEY

FROM: JACQUELINE ATKINS

DATE: 10/9/92

NUMBER OF PAGES: 1

FAX (310) 203-3852

PHONE (310) 203-3959

A Professor at UCLA told me that you might be able to give me the answer to: What is the 40,000th digit of Pi?

We would like to use the answer in our show. Can you help?

The Borwein-Plouffe Observation

In 1996, Peter Borwein and Simon Plouffe observed that the following well-known formula for $\log_e 2$

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{n 2^n} = 0.69314718055994530942\ldots$$

leads to a simple scheme for computing binary digits at an arbitrary starting position (here {} denotes fractional part):

$$\begin{aligned} \left\{2^d \log 2\right\} &= \left\{\sum_{n=1}^{d} \frac{2^{d-n}}{n}\right\} + \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \\ &= \left\{\sum_{n=1}^{d} \frac{2^{d-n} \bmod n}{n}\right\} + \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \end{aligned}$$

Fast Exponentiation Mod n

The exponentiation (2^{d-n} mod n) in this formula can be evaluated very rapidly by means of the binary algorithm for exponentiation, performed modulo n:

Example problem: Calculate the last digit of 3^{17} (i.e., compute 3^{17} mod 10).

Algorithm A: 3x3x3x3x3x3x3x3x3x3x3x3x3x3x3x3x3 = 129140163. Ans =3.

Algorithm B: $3^{17} = (((3^2)^2)^2)^2 \times 3$ = 129140163. Ans = 3.

Algorithm C: Same as Algorithm B, but reduce mod 10 after each multiply operation:

3^2 mod 10 = 9; 9^2 mod 10 = 1; 1^2 mod 10 = 1; 1^2 mod 10 = 1; 1 x 3 = 3. Ans = 3.

Note that with Algorithm C, we never have to deal with integers greater than 81. This is a huge savings when we deal with very large powers.

The BBP Formula for Pi

In 1996, Simon Plouffe used DHB's PSLQ program and high-precision arithmetic software to discover this new 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 was found by searching for integer relations between pi and about 25 other constants with known series formulas like log(2).

This formula permits one to compute binary (or hexadecimal) digits of pi beginning at an arbitrary starting position.

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

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.

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.

Some Other BBP-Type Formulas

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

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

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

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

Papers by D. H. Bailey, P. B. Borwein, S. Plouffe, D. Broadhurst and R. Crandall.

Normality (Digit Randomness) of Mathematical Constants

A real number x is said to be b-normal (or normal base b) if every m-long string of base-b digits appears, in the limit, with frequency b^{-m}.

Whereas it can be shown that almost all real numbers are b-normal (for any b), there are only a handful of proven explicit examples.

It is still not known whether any of the following are b-normal for any b:

$$\begin{aligned}
\sqrt{2} &= 1.4142135623730950488\ldots \\
\phi = \frac{\sqrt{5}-1}{2} &= 0.6180339887498948482\ldots \\
\pi &= 3.1415926535897932385\ldots \\
e &= 2.7182818284590452354\ldots \\
\log 2 &= 0.6931471805599453094\ldots \\
\log 10 &= 2.3025850929940456840\ldots \\
\zeta(2) &= 1.6449340668482264365\ldots \\
\zeta(3) &= 1.2020569031595942854\ldots
\end{aligned}$$

A Connection Between BBP Formulas and Normality

Let {} denote fractional part. Consider the sequence defined by $x_0 = 0$,

$$x_n = \left\{ 2x_{n-1} + \frac{1}{n} \right\}$$

Result: log(2) is 2-normal if and only if this sequence is equidistributed in the unit interval.

In a similar vein, consider the sequence $x_0 = 0$, and

$$x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\}$$

Result: pi is 16-normal if and only if this sequence is equidistributed in the unit interval.

A similar result holds for any constant that possesses a BBP-type formula.

D. H. Bailey and R. E. Crandall, "On the Random Character of Fundamental Constant Expansions," *Experimental Mathematics*, vol. 10, no. 2 (Jun 2001), pg. 175-190.

A Class of Provably Normal Constants

We have also shown that this constant (among many others) is 2-normal:

$$\begin{aligned}\alpha_{2,3} &= \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}} = \frac{1}{3 \cdot 2^3} + \frac{1}{3^2 \cdot 2^{3^2}} + \frac{1}{3^3 \cdot 2^{3^3}} + \frac{1}{3^4 \cdot 2^{3^4}} \cdots \\ &= 0.0418836808315029850712528986245716824260 96\ldots_{10} \\ &= 0.0\mathrm{AB8E38F684BDA12F684BF35BA781948B0FCD6E9E0}\ldots_{16}\end{aligned}$$

This means, for instance, that the entire works of William Shakespeare are contained, in coded form, in the base-16 digits of this number.

These results have led to a practical and efficient pseudo-random number generator based on the binary digits of alpha.

1. D. H. Bailey and R. E. Crandall, “Random Generators and Normal Numbers,” *Experimental Mathematics*, vol. 11, no. 4 (2002), pg. 527-546.
2. D. H. Bailey, "A Pseudo-Random Number Generator Based on Normal Numbers," manuscript, Dec 2004, http://crd.lbl.gov/~dhbailey/dhbpapers/normal-random.pdf.

The "Hot Spot" Lemma for Proving Normality

We are now able to prove normality for these alpha constants very simply, by means of a new result that we call the "hot spot" lemma, proven using ergodic theory:

Hot Spot Lemma: Let {} denote fractional part. Then x is b-normal if and only if there is no y in [0,1) such that

$$\liminf_{m\to\infty} \limsup_{n\to\infty} \frac{\#_{0\le j<n}(|\{b^j x\} - y| < b^{-m})}{2nb^{-m}} = \infty$$

Paraphrase: x is b-normal if and only if it has no base-b hot spots.

Sample Corollary: If, for each m and n, no m-long string of digits appears in the first n digits of the base-2 expansion of x more often than 1,000 n 2^{-m} times, then x is 2-normal.

D. H. Bailey and M. Misiurewicz, "A Strong Hot Spot Theorem," *Proceedings of the American Mathematical Society*, vol. 134 (2006), no. 9, pg. 2495-2501.

A Curious Observation

About 12 years ago, Peter Borwein asked me to calculate numerical values of the definite integrals of the form

$$I = \int_0^\infty f(t) e^{-t^2/2} \, dt$$

In doing these computations I was surprised to find that the results were remarkably accurate, even when using just a simple block-function or trapezoidal rule approximation, with only a modest number of grid points.

Why is this?

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.

K. Atkinson, *An Introduction to Numerical Analysis*, John Wiley, 1989, pg. 289.

The Tanh-Sinh Algorithm for Numerical Integration

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

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

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 such functions, the Euler-Maclaurin formula of numerical analysis implies that the simple summation above is remarkably accurate. Reducing h by half typically doubles the number of correct digits.

Tanh-sinh quadrature is the best integration scheme for functions with vertical derivatives or blow-up singularities at endpoints, or for any function at very high precision (> 1000 digits).

1. D. H. Bailey, X. S. Li and K. 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.

Example Application of Tanh-Sinh Integration

The following integral cannot be evaluated symbolically by either *Maple* (version 11) or *Mathematica* (version 6.0):

$$\int_0^{\pi/2} \frac{\arcsin(\sqrt{2}/2 \cdot \sin x) \sin x \, dx}{\sqrt{4 - 2\sin^2 x}} =$$
$$0.38494647276779467737973363453435093937863 7\ldots$$

However, by employing tanh-sinh quadrature (which produces the numerical value shown above) followed by the Inverse Symbolic Calculator (ISC 2.0), available at `http://ddrive.cs.dal.ca/~isc,` one obtains

$$\int_0^{\pi/2} \frac{\arcsin(\sqrt{2}/2 \cdot \sin x) \sin x \, dx}{\sqrt{4 - 2\sin^2 x}} = \frac{\sqrt{2}\pi \log 2}{8}$$

This has been numerically verified to over 1000-digit precision.

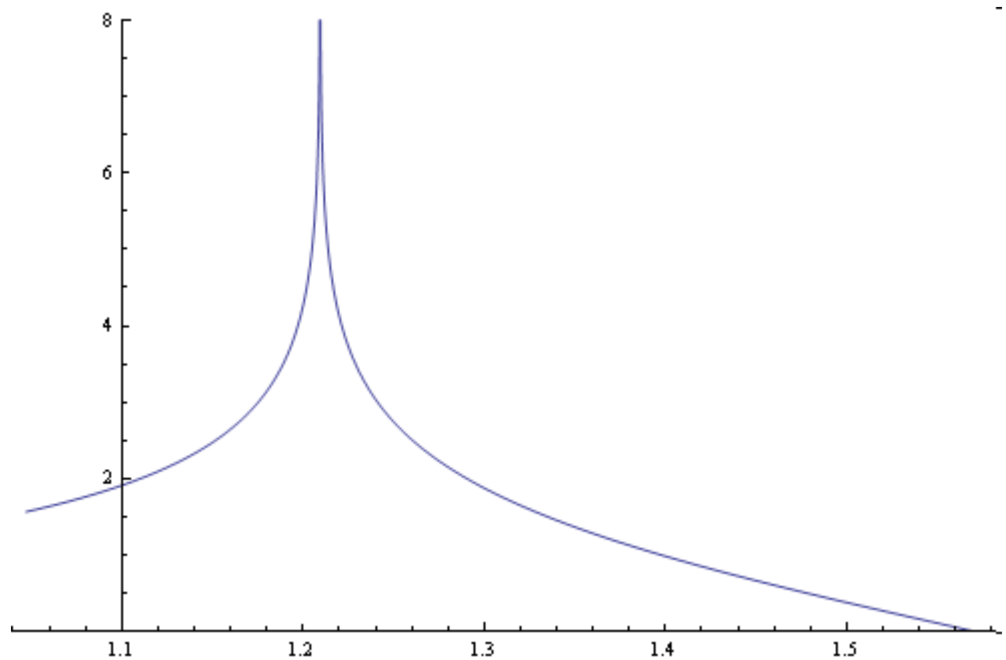
A Log-Tan Integral Identity from Mathematical Physics

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

This conjectured identity arises in mathematical physics from analysis of volumes of ideal tetrahedra in hyperbolic space.

We have verified this numerically to 20,000 digits using highly parallel tanh-sinh quadrature, but no formal proof is known.

D. H. Bailey, J. M. Borwein, V. Kapoor and E. Weisstein, “Ten Problems in Experimental Mathematics,” *American Mathematical Monthly*, vol. 113, no. 6 (Jun 2006), pg. 481-409 .



Parallel Evaluation of the log-tan Integral

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \;=\; 1.15192547054449104710\ldots$$

CPUs	Init	Integral #1	Integral #2	Total	Speedup
1	190013	1534652	1026692	2751357	1.00
16	12266	101647	64720	178633	15.40
64	3022	24771	16586	44379	62.00
256	770	6333	4194	11297	243.55
1024	199	1536	1034	2769	993.63

1-CPU timings are sums of timings from a 64-CPU run, where barrier waits and communication were not timed.

The performance rate for the 1024-CPU run is 690 Gflop/s.

D. H. Bailey and J. M. Borwein, “Highly Parallel, High-Precision Numerical Integration,” *International Journal of Computational Science and Engineering*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/quadparallel.pdf.

Integrals from Ising Theory of Mathematical Physics

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

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

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

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

where (in the last line) $$u_k = \prod_{i=1}^k t_i$$

D. H. Bailey, 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.

Computing and Evaluating C_n

We first showed that the multi-dimensional C_n integrals can be transformed to much more manageable 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 the following results and others were found, then proven:

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

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 number? We copied the first 50 digits of this numerical value into the online Inverse Symbolic Calculator (ISC), now available at

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

The result was:

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

where gamma denotes Euler's constant. This result is now proven and has been generalized to an asymptotic expansion.

Other Ising Integral Evaluations

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

where Li denotes the polylogarithm function.

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 3-D integral to 250-digit precision, using a parallel high-precision 3-D quadrature program. Then we used PSLQ 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\,dy\,dz
\end{aligned}
$$

Recursions in Ising Integrals

Consider the 2-parameter class of Ising integrals

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

(which have connections to quantum field theory). After computing 1000-digit numerical values for all n <= 36 and all k <= 75 (2660 individual quadrature calculations, performed in parallel), and applying PSLQ, we found linear relations in the rows of this array. For example, when n = 3:

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

These recursions have been proven for n = 1, 2, 3, 4. Similar, but more complicated, recursions have been found for larger n (see next page).

D. H. Bailey, D. Borwein, J. M. Borwein and R. E. Crandall, “Hypergeometric Forms for Ising-Class Integrals,” *Experimental Mathematics*, vol. 16 (2007), no. 3, pg. 257-276.

Experimental Recursion for n = 24

$$
\begin{aligned}
0 \stackrel{?}{=} \; & C_{24,1} \\
& -1107296298\, C_{24,3} \\
& +1288574336175660\, C_{24,5} \\
& -88962910652291256000\, C_{24,7} \\
& +1211528914846561331193600\, C_{24,9} \\
& -5367185923241422152980553600\, C_{24,11} \\
& +9857686103738772925980190636800\, C_{24,13} \\
& -8476778037073141951236532459008000\, C_{24,15} \\
& +3590120926882411593645052529049600000\, C_{24,17} \\
& -745759114781380983188217871663104000000\, C_{24,19} \\
& +71215552121869985477578381170258739200000\, C_{24,21} \\
& -2649853457247995406113355087174696960000000\, C_{24,23} \\
& +24912519234220575094208313195233280000000000\, C_{24,25}
\end{aligned}
$$

Jonathan Borwein and Bruno Salvy have now given an explicit form for these recursions, together with code to compute any desired case.

J. M. Borwein and B. Salvy, "A Proof of a Recursion for Bessel Moments," *Experimental Mathematics*, to appear, 2008, http://users.cs.dal.ca/~jborwein/recursion.pdf.

Some Results from a New Study of Bessel Moments (Mar. 2008)

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

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

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

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

where F denotes Gauss' hypergeometric function, and $c_{n,k} = n!\, k!\, 2^{-n} C_{n,k}$.

These and numerous other results are available in a new paper on Bessel moments, which have application not only in Ising theory, but also in quantum field theory, condensed matter theory and "diamond lattice" walks.

D. H. Bailey, J. M. Borwein, D. Broadhurst and M. L. Glasser, "Elliptic Integral Evaluations of Bessel Moments," *Journal of Physics A*, vol. 41 (2008), pg. 205203, http://crd.lbl.gov/~dhbailey/dhbpapers/b3g.pdf.

Some Other New Indentities Found in Bessel Moment Study

$$
\begin{aligned}
C_{5,0} - 10C_{3,2} + 5C_{1,4} &= 0 \\
\sum_{m=0}^{\lfloor n/2 \rfloor} (-1)^m \binom{n}{2m} \int_0^\infty t^{n-2k} [\pi I_0(t)]^{n-2m} [K_0(t)]^{n+2m} \, dt &= 0 \\
\frac{\pi}{4} \sum_{n=0}^{\infty} \left(\frac{(2n)!}{2^{2n} n!} \right)^3 \sum_{m=0}^{n} 2^{2m} \frac{{}_2F_1\left(\begin{array}{c} 2n+1, 2n+1 \\ 2n+2+m \end{array} \middle| \frac{1}{2} \right)}{(n-m)!(2n+1+m)!} &= \frac{\pi^2}{4\sqrt{3}} \, {}_3F_2\left(\begin{array}{c} \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ 1, 1 \end{array} \middle| \frac{1}{4} \right)
\end{aligned}
$$

The first identity has been numerically verified to 14,285-digit precision.

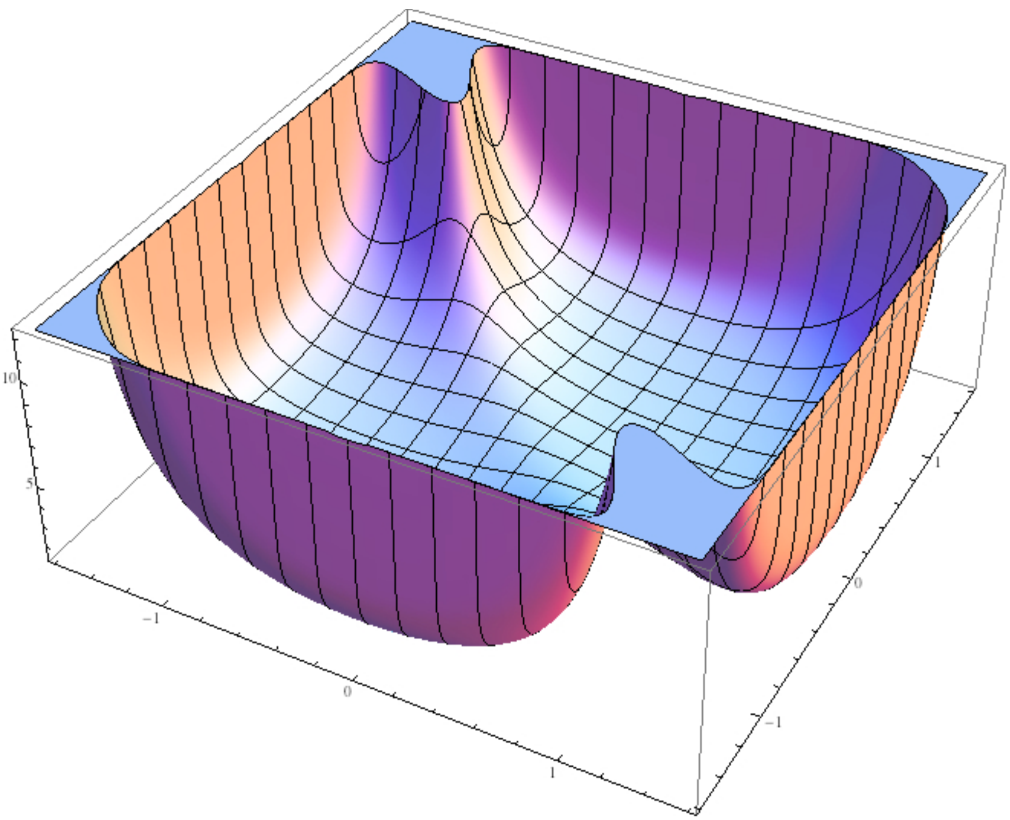
The second identity holds for every pair of integers (n,k) with 2*k in [2, n].

The Bessel moment paper gives analytic evaluations of all definite integrals involving products up to six Bessel functions. A computational-experimental methodology was employed throughout the process:

D. H. Bailey, J. M. Borwein, D. Broadhurst and M. L. Glasser, “Elliptic Integral Evaluations of Bessel Moments,” *Journal of Physics A*, vol. 41 (2008), pg. 205203, available at http://crd.lbl.gov/~dhbailey/dhbpapers/b3g.pdf.

An Example of Computations Involved in the Bessel Moment Study

$$
\begin{aligned}
c_{5,0} &= \frac{\pi}{2}\int_{-\pi/2}^{\pi/2}\int_{-\pi/2}^{\pi/2}\frac{\mathbf{K}(\sin\theta)\,\mathbf{K}(\sin\phi)}{\sqrt{\cos^2\theta\cos^2\phi+4\sin^2(\theta+\phi)}}\,d\theta\,d\phi\,d\phi \\
&= 135.26830258086883759422627964619220742030588935942352678469\ldots
\end{aligned}
$$



Cautionary Example

These constants agree to 42 decimal digit accuracy, but are NOT equal:

$$\int_0^\infty \cos(2x) \prod_{n=0}^{\infty} \cos(x/n)\, dx \quad = \quad 0.39269908169872415480783042290993786052464543418723\ldots$$

$$\frac{\pi}{8} \quad = \quad 0.39269908169872415480783042290993786052464617492189\ldots$$

Richard Crandall has now shown that this integral is merely the first term of a very rapidly convergent series that converges to pi/8:

$$\frac{\pi}{8} \;=\; \sum_{m=0}^{\infty} \int_0^\infty \cos(2(2m+1)x) \prod_{n=0}^{\infty} \cos(x/n)\, dx$$

1. D. H. Bailey, J. M. Borwein, V. Kapoor and E. Weisstein, “Ten Problems in Experimental Mathematics,” *American Mathematical Monthly*, vol. 113, no. 6 (Jun 2006), pg. 481-409 .

2. R. E. Crandall, “Theory of ROOF Walks, 2007, available at http://people.reed.edu/~crandall/papers/ROOF.pdf

Summary

- Due to seminal early contributions by researchers such as Peter Borwein, tremendous progress has been made recently in experimental math.
- Software-based facilites now permit even very complicated computations to be performed with high levels of precision, requiring only minor modification to existing computer programs.
- Symbolic computing tools continue to advance in sophistication and usability.
- Continued rapid progress is very likely, due both to the inexorable upward march of Moore's Law, and also to an influx of young researchers highly skilled in computing.

This talk is available at:

`http://crd.lbl.gov/~dhbailey/dhbtalks/dhb-peter-borwein.pdf`