

## Experimental Mathematics: Tools of the Trade

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This talk is available at:

http://crd.lbl.gov/~dhbailey/dhbtalks/dhb-expmath-tools.pdf



## Computational Methods Used in Experimental Mathematics



- Symbolic computation for algebraic and calculus manipulations.
- Integer-relation methods, especially the "PSLQ" algorithm.
- High-precision integer and floating-point arithmetic.
- High-precision evaluation of integrals and infinite series summations.
- The Wilf-Zeilberger algorithm for proving summation identities.
- Iterative approximations to continuous functions.
- Identification of functions based on graph characteristics.
- Graphics and visualization methods targeted to mathematical objects.
- Highly parallel implementations of the above algorithms.

#### Arbitrary Precision Arithmetic: The "Electron Microscope" of Computer Math



- High-precision integer arithmetic is required in symbolic computing packages.
- High-precision floating-point arithmetic is required to permit identification of mathematical constants using PSLQ or online constant recognition facilities.
- The most common requirement is for 200-500 digits, although thousands of digits are sometimes required.
- One problem required 50,000-digit arithmetic.

## Schemes for High-Precision Floating-Point Arithmetic



- A high-precision number is typically represented as a string of n + 4 integers (or a string of n + 4 floating-point numbers with integer values):
  - First two words give sign and "exponent."
  - The next n words contain the mantissa (say 48 bits per word).
  - The two end words are used for "scratch space" in certain operations.
- For basic arithmetic operations, straightforward adaptions of elementary schemes suffice up to about 1000 digits. Arithmetic is typically performed base 2<sup>32</sup> or 2<sup>48</sup> instead of base 10.
- Beyond about 1000 digits, Karatsuba's algorithm or FFTs can be used for significantly faster multiply performance.
- Division and square roots can be performed by Newton iterations.
- For transcendental functions, Taylor's series evaluations or (at higher precision levels) quadratically convergent algorithms are used.

### 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."

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

Other widely used high-precision software:

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

David H. Bailey, Yozo Hida, Xiaoye S. Li and Brandon Thompson, "ARPREC: An Arbitrary Precision Computation Package," manuscript, Sept 2002, http://crd.lbl.gov/~dhbailey/dhbpapers/arprec.pdf.



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

$$a_1x_1 + a_2x_2 + \dots + a_nx_n = 0$$

(or within "epsilon" of zero, where epsilon = 10<sup>-p</sup> 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*.

A "multi-pair" variant of PSLQ has been found that is well-suited for parallel computation.

 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.
 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.

## **PSLQ**, Continued



- PSLQ constructs a sequence of integer-valued matrices B<sub>n</sub> that reduces the vector y = x \* B<sub>n</sub>, until either the relation is found (as one of the columns of B<sub>n</sub>), or else precision is exhausted.
- At the same time, PSLQ generates a steadily growing bound on the size of any possible relation.
- When a relation is found, the size of smallest entry of the vector y suddenly drops to roughly "epsilon" (i.e. 10<sup>-p</sup>, where p is the number of digits of precision).
- The size of this drop can be viewed as a "confidence level" that the relation is real and not merely a numerical artifact -- a drop of 20+ orders of magnitude almost always indicates a real relation.
- 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<sub>k</sub>), both in the input data and in the operation of the algorithm.



## Application of PSLQ: Bifurcation Points in Chaos Theory

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

3.54409035955192285361596598660480454058309984544457367545781...

Applying PSLQ to the vector (1, t, t<sup>2</sup>, t<sup>3</sup>, ..., t<sup>12</sup>), one finds that t is a root of  $0 = 4913 + 2108t^{2} - 604t^{3} - 977t^{4} + 8t^{5} + 44t^{6} + 392t^{7}$   $-193t^{8} - 40t^{9} + 48t^{10} - 12t^{11} + t^{12}$ 

J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, A.K. Peters, 2004, pg. 50.

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## Some Supercomputer-Class PSLQ Solutions



- Identification of B<sub>4</sub>, 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. 1000-digit arithmetic. Run on Apple-based parallel 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.

But in most problems the dominant cost is computing the constants involved.

- 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*, to appear, 2007, http://crd.lbl.gov/~dhbailey/dhbpapers/meijer.pdf.



In 1996, Peter Borwein and Simon Plouffe observed that the following well-known formula for  $\log_{\rm e} 2$ 

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{n2^n} = 0.69314718055994530942\dots$$

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

$$\left\{ 2^{d} \log 2 \right\} = \left\{ \sum_{n=1}^{d} \frac{2^{d-n}}{n} \right\} + \sum_{\substack{n=d+1 \\ n=d+1}}^{\infty} \frac{2^{d-n}}{n}$$
$$= \left\{ \sum_{n=1}^{d} \frac{2^{d-n} \mod n}{n} \right\} + \sum_{\substack{n=d+1 \\ n=d+1}}^{\infty} \frac{2^{d-n}}{n}$$



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

Simple example problem: Calculate the 3<sup>17</sup> mod 10.

Note that with Algorithm C, we never have to deal with integers > 81.

## The BBP Formula for Pi



In 1996, Simon Plouffe used DHB's PSLQ program and arbitrary precision 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 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 pi, except  $n = 2^{m}$ .

 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.
 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.

## **Proof of the BBP Formula**



$$\int_{0}^{1/\sqrt{2}} \frac{x^{j-1} dx}{1-x^8} = \int_{0}^{1/\sqrt{2}} \sum_{k=0}^{\infty} x^{8k+j-1} dx = \frac{1}{2^{j/2}} \sum_{k=0}^{\infty} \frac{1}{16^k (8k+j)}$$

Thus

$$\begin{split} \sum_{k=0}^{\infty} \frac{1}{16^k} \left( \frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6} \right) \\ &= \int_0^{1/\sqrt{2}} \frac{(4\sqrt{2} - 8x^3 - 4\sqrt{2}x^4 - 8x^5) \, dx}{1 - x^8} \\ &= \int_0^1 \frac{16(4 - 2y^3 - y^4 - y^5) \, dy}{16 - y^8} \\ &= \int_0^1 \frac{16(y - 1) \, dy}{(y^2 - 2)(y^2 - 2y + 2)} \\ &= \int_0^1 \frac{4y \, dy}{y^2 - 2} - \int_0^1 \frac{(4y - 8) \, dy}{y^2 - 2y + 2} \\ &= \pi \end{split}$$

## **Some Other BBP-Type Identities**



$$\begin{split} \pi^2 &= \frac{1}{8} \sum_{k=0}^{\infty} \frac{1}{64^k} \left( \frac{144}{(6k+1)^2} - \frac{216}{(6k+2)^2} - \frac{72}{(6k+3)^2} - \frac{54}{(6k+4)^2} + \frac{9}{(6k+5)^2} \right) \\ \pi^2 &= \frac{2}{27} \sum_{k=0}^{\infty} \frac{1}{729^k} \left( \frac{243}{(12k+1)^2} - \frac{405}{(12k+2)^2} - \frac{81}{(12k+4)^2} - \frac{27}{(12k+5)^2} \right) \\ &- \frac{72}{(12k+6)^2} - \frac{9}{(12k+7)^2} - \frac{9}{(12k+8)^2} - \frac{5}{(12k+10)^2} + \frac{1}{(12k+11)^2} \right) \\ \zeta(3) &= \frac{1}{1792} \sum_{k=0}^{\infty} \frac{1}{2^{12k}} \left( \frac{6144}{(24k+1)^3} - \frac{43008}{(24k+2)^3} + \frac{24576}{(24k+3)^3} + \frac{30720}{(24k+4)^3} \right) \\ &- \frac{1536}{(24k+5)^3} + \frac{3072}{(24k+6)^3} + \frac{768}{(24k+7)^3} - \frac{3072}{(24k+9)^3} - \frac{2688}{(24k+10)^3} \\ &- \frac{192}{(24k+11)^3} - \frac{1536}{(24k+12)^3} - \frac{96}{(24k+13)^3} - \frac{672}{(24k+14)^3} - \frac{384}{(24k+15)^3} \\ &+ \frac{24}{(24k+17)^3} + \frac{48}{(24k+18)^3} - \frac{12}{(24k+19)^3} + \frac{120}{(24k+20)^3} + \frac{48}{(24k+21)^3} \\ &- \frac{42}{(24k+22)^3} + \frac{3}{(24k+23)^3} \right) \\ &= \frac{25}{2} \log \left( \frac{781}{256} \left( \frac{57-5\sqrt{5}}{57+5\sqrt{5}} \right)^{\sqrt{5}} \right) \\ &= \sum_{k=0}^{\infty} \frac{1}{5^{5k}} \left( \frac{5}{5k+2} + \frac{1}{5k+3} \right) \end{split}$$

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



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<sup>-m</sup>.

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:

$$\begin{split} \sqrt{2} &= 1.4142135623730950488\dots \\ \phi &= \frac{\sqrt{5}-1}{2} &= 0.61803398874989484820\dots \\ \pi &= 3.1415926535897932385\dots \\ e &= 2.7182818284590452354\dots \\ \log 2 &= 0.69314718055994530942\dots \\ \log 10 &= 2.3025850929940456840\dots \\ \zeta(2) &= 1.6449340668482264365\dots \\ \zeta(3) &= 1.2020569031595942854\dots \end{split}$$

## 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.



We have also shown that the following constant is 2-normal:

$$\begin{aligned} \alpha_{2,3} &= \sum_{k=1}^{\infty} \frac{1}{3^k 2^{3^k}} \\ &= 0.041883680831502985071252898624571682426096\dots_{10} \end{aligned}$$

= 0.0AB8E38F684BDA12F684BF35BA781948B0FCD6E9E0...16

This was originally proven by Stoneham in 1970, but we have generalized this to case where (2,3) is replaced by any relatively prime pair > 2. We have also extended this to an uncountably infinite class.

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

<sup>1.</sup> D. H. Bailey and R. E. Crandall, "Random Generators and Normal Numbers," *Experimental Mathematics*, vol. 11, no. 4 (2002), pg. 527-546.

<sup>2.</sup> 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.

## The Euler-Maclaurin Formula and Infinite Series Summation



The Euler-Maclaurin summation formula approximates a finite sum as an integral with high-order corrections:

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

[Here h = (b - a)/n, x<sub>j</sub> = a + j h, B<sub>2k</sub> are Bernoulli numbers, and D<sup>m</sup> f(x) means m-th derivative of f.]

One can use the E-M to compute a high-precision sum for an infinite series: Explicitly compute, to high precision, the sum of the first N terms of the series, where N = 10<sup>p</sup> (we typically set p = 8, so that N = 100,000,000). Then use the E-M formula to calculate a high-precision value for the "tail." Each term of the E-M formula adds roughly p more correct digits.

D. H. Bailey, et. al, *Experimental Mathematics in Action*, A.K. Peters, 2007, pg. 63-70.

#### Example: Computing Catalan's Constant to High Precision



$$G = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2}$$
  
= 0.91596559417721901505460351493238411077414937...

Let  $f(x) = (2x+1) / [(4x+1)^2 (4x+3)^2]$ . Then for  $n = 10^6$  we can write

$$G = (1 - 1/3^2) + (1/5^2 - 1/7^2) + (1/9^2 - 1/11^2) + \cdots$$
  
=  $8 \sum_{k=0}^{\infty} \frac{2k+1}{(4k+1)^2(4k+3)^2}$   
=  $8 \sum_{k=0}^{n} \frac{2k+1}{(4k+1)^2(4k+3)^2} + 8 \sum_{k=n+1}^{\infty} \frac{2k+1}{(4k+1)^2(4k+3)^2}$   
=  $8 \sum_{k=0}^{n} \frac{2k+1}{(4k+1)^2(4k+3)^2} + 8 \int_{n+1}^{\infty} f(x) \, dx + 4f(n+1)$   
 $-8 \sum_{i=1}^{m} \frac{B_{2i}}{(2i)!} f^{(2i-1)}(n+1) + 8E$ 

#### **Euler's Transformation for Summing Alternating Infinite Series**



$$\sum_{k=0}^{\infty} (-1)^{k} u_{k} = \sum_{m=0}^{n-1} (-1)^{k} u_{k} + \sum_{k=0}^{\infty} \frac{(-1)^{k} \Delta^{k} u_{n}}{2^{k+1}}$$

$$\Delta^{1} u_{n} = u_{n+1} - u_{n}$$

$$\Delta^{2} u_{n} = \Delta^{1} u_{n+1} - \Delta^{1} u_{n} = u_{n+2} - 2u_{n+1} + u_{n}$$

$$\Delta^{3} u_{n} = \Delta^{2} u_{n+2} - \Delta^{2} u_{n+1} = u_{n+3} - 3u_{n+2} + 3u_{n+1} - u_{n}$$

For example, Catalan's constant can be computed to 500-digit precision by setting n = 1000, then evaluating 400 terms of the second series (a total of 1400 function evaluations).

William H. Press, et al, Numerical Recipes, Cambridge University Press, 1966, pg. 133-134.

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### Converting All-Positive Series to Alternating Series



Given an all-positive series  $(x_n)$ , one can construct an alternating series  $(y_n)$  with the same sum as follows: Set  $y_0 = x_0$ , then for n > 0

$$y_n = (-1)^n \sum_{k=0}^{\infty} 2^k x_{n2^k}$$

Each of these individual summations converges quite rapidly, so only a modest number of terms typically need to be computed. Euler's transformation can then be applied to find the sum

$$S = \sum_{n=0}^{\infty} y_n = \sum_{n=0}^{\infty} x_n$$

This method works fairly well, but is many times more costly than the alternating series case. Is there an efficient, general-purpose, numerically robust scheme for finding high-precision values for infinite series sums?



In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of Jonathan Borwein the result

$$\sum_{k=1}^{\infty} \left( 1 + \frac{1}{2} + \dots + \frac{1}{k} \right)^2 k^{-2} = 4.59987 \dots \approx \frac{17}{4} \zeta(4) = \frac{17\pi^4}{360}$$

Borwein was very skeptical, but subsequent computations affirmed this to high precision. This is a special case of the following class:

$$\zeta(s_1, s_2, \cdots, s_k) = \sum_{n_1 > n_2 > \cdots > n_k > 0} \prod_{j=1}^k n_j^{-|s_j|} \sigma_j^{-n_j},$$

where  $s_j$  are integers and  $\sigma_j$  = sign of  $s_j$ . These can be rapidly computed using the online tool http://www.cecm.sfu.ca/projects/ezface+.

1. J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, A.K. Peters, 2004, pg. 56.

2. J. M. Borwein and D. H. Bailey, *Experimentation in Mathematics*, A.K. Peters, 2004, pg 142-160.

## **Multivariate Zeta Example**



Consider this example:

$$S_{2,3} = \sum_{\substack{k=1 \\ k=1}}^{\infty} \left( 1 - \frac{1}{2} + \dots + (-1)^{k+1} \frac{1}{k} \right)^2 (k+1)^{-3}$$
$$= \sum_{\substack{0 < i, j < k \\ k>0}} \frac{(-1)^{i+j+1}}{ijk^3} = -2\zeta(3, -1, -1) + \zeta(3, 2)$$

Using the EZFACE+ tool, we obtain the numerical value:

0.1561669333811769158810359096879881936857767098403038729 57529354497075037440295791455205653709358147578...

Using PSLQ, we then found this evaluation:

$$S_{2,3} = 4 \operatorname{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30} \log^5(2) - \frac{17}{32}\zeta(5) - \frac{11}{720}\pi^4 \log(2) + \frac{7}{4}\zeta(3) \log^2(2) + \frac{1}{18}\pi^2 \log^3(2) - \frac{1}{8}\pi^2 \zeta(3)$$

## Evaluation of Ten Constants from Quantum Field Theory









J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, A.K. Peters, 2004, pg. 58.

 $V_{1} = 6\zeta(3) + 3\zeta(4)$   $V_{2A} = 6\zeta(3) - 5\zeta(4)$   $V_{2N} = 6\zeta(3) - \frac{13}{2}\zeta(4) - 8U$   $V_{3T} = 6\zeta(3) - 9\zeta(4)$   $V_{3S} = 6\zeta(3) - \frac{11}{2}\zeta(4) - 4C^{2}$   $V_{3L} = 6\zeta(3) - \frac{15}{4}\zeta(4) - 6C^{2}$   $V_{4A} = 6\zeta(3) - \frac{77}{12}\zeta(4) - 6C^{2}$   $V_{4N} = 6\zeta(3) - 14\zeta(4) - 16U$ 

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

where

$$C = \sum_{k>0} \sin(\pi k/3)/k^2$$
  

$$U = \sum_{j>k>0} \frac{(-1)^{j+k}}{j^3 k}$$
  

$$V = \sum_{j>k>0} (-1)^j \cos(2\pi k/3)/(j^3 k)$$

## **PSLQ and Sculpture**



The complement of the figure-eight knot, when viewed in hyperbolic space, has finite volume

#### 2.029883212819307250042...

Recently physicist David Broadhurst found, using PSLQ, that this constant is given by the formula:

$$V = \frac{\sqrt{3}}{9} \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n} \left( \frac{18}{(6n+1)^2} - \frac{18}{(6n+2)^2} - \frac{24}{(6n+3)^2} - \frac{6}{(6n+4)^2} + \frac{2}{(6n+5)^2} \right)$$

and thus is a base-3 BBP-type constant.

J. M. Borwein and D. H. Bailey, *Mathematics by Experiment*, A.K. Peters, 2004, pg. 53.



## **New Ramanujan-Like Identities**



Guillera has recently found some Ramanujan-like identities, including:

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (13 + 180n + 820n^2) \left(\frac{1}{32}\right)^{2n}$$
  
$$\frac{32}{\pi^2} = \sum_{n=0}^{\infty} (-1)^n r(n)^5 (1 + 8n + 20n^2) \left(\frac{1}{2}\right)^{2n}$$
  
$$\frac{32}{\pi^3} = \sum_{n=0}^{\infty} r(n)^7 (1 + 14n + 76n^2 + 168n^3) \left(\frac{1}{32}\right)^{2n}.$$

where

$$r(n) = \frac{(1/2)_n}{n!} = \frac{1/2 \cdot 3/2 \cdot \dots \cdot (2n-1)/2}{n!} = \frac{\Gamma(n+1/2)}{\sqrt{\pi} \Gamma(n+1)}$$

Guillera proved the first two of these using the Wilf-Zeilberger algorithm. He ascribed the third to Gourevich, who found it using integer relation methods. Are there any higher-order analogues?

#### PSLQ Searches for Additional Formulas



We searched for additional formulas of either the following forms:

$$\frac{c}{\pi^m} = \sum_{n=0}^{\infty} r(n)^{2m+1} (p_0 + p_1 n + \dots + p_m n^m) \alpha^{2n}$$
$$\frac{c}{\pi^m} = \sum_{n=0}^{\infty} (-1)^n r(n)^{2m+1} (p_0 + p_1 n + \dots + p_m n^m) \alpha^{2n}.$$

where c is some linear combination of 1,  $2^{1/2}$ ,  $2^{1/3}$ ,  $2^{1/4}$ ,  $2^{1/6}$ ,  $4^{1/3}$ ,  $8^{1/4}$ ,  $32^{1/6}$ ,  $3^{1/2}$ ,  $3^{1/3}$ ,  $3^{1/4}$ ,  $3^{1/6}$ ,  $9^{1/3}$ ,  $27^{1/4}$ ,  $243^{1/6}$ ,  $5^{1/2}$ ,  $5^{1/4}$ ,  $125^{1/4}$ ,  $7^{1/2}$ ,  $13^{1/2}$ ,  $6^{1/2}$ ,  $6^{1/3}$ ,  $6^{1/4}$ ,  $6^{1/6}$ , 7,  $36^{1/3}$ ,  $216^{1/4}$ ,  $7776^{1/6}$ ,  $12^{1/4}$ ,  $108^{1/4}$ ,  $10^{1/2}$ ,  $10^{1/4}$ ,  $15^{1/2}$ 

where each of the coefficients  $p_i$  is a linear combination of 1,  $2^{1/2}$ ,  $3^{1/2}$ ,  $5^{1/2}$ ,  $6^{1/2}$ ,  $7^{1/2}$ ,  $10^{1/2}$ ,  $13^{1/2}$ ,  $14^{1/2}$ ,  $15^{1/2}$ ,  $30^{1/2}$  and where alpha is chosen as one of the following: 1/2, 1/4, 1/8, 1/16, 1/32, 1/64, 1/128, 1/256,  $\sqrt{5} - 2$ ,  $(2 - \sqrt{3})^2$ ,  $5\sqrt{13} - 18$ ,  $(\sqrt{5} - 1)^4/128$ ,  $(\sqrt{5} - 2)^4$ ,  $(2^{1/3} - 1)^4/2$ ,  $1/(2\sqrt{2})$ ,  $(\sqrt{2} - 1)^2$ ,  $(\sqrt{5} - 2)^2$ ,  $(\sqrt{3} - \sqrt{2})^4$ 

# Relations Found by PSLQ (in addition to Guillera's three relations)



$$\begin{aligned} \frac{4}{\pi} &= \sum_{n=0}^{\infty} r(n)^3 (1+6n) \left(\frac{1}{2}\right)^{2n} \\ \frac{16}{\pi} &= \sum_{n=0}^{\infty} r(n)^3 (5+42n) \left(\frac{1}{8}\right)^{2n} \\ \frac{12^{1/4}}{\pi} &= \sum_{n=0}^{\infty} r(n)^3 (-15+9\sqrt{3}-36n+24\sqrt{3}n) \left(2-\sqrt{3}\right)^{4n} \\ \frac{32}{\pi} &= \sum_{n=0}^{\infty} r(n)^3 (-1+5\sqrt{5}+30n+42\sqrt{5}n) \left(\frac{(\sqrt{5}-1)^4}{128}\right)^{2n} \\ \frac{5^{1/4}}{\pi} &= \sum_{n=0}^{\infty} r(n)^3 (-525+235\sqrt{5}-1200n+540\sqrt{5}n) \left(\sqrt{5}-2\right)^{8n} \\ \frac{2\sqrt{2}}{\pi} &= \sum_{n=0}^{\infty} (-1)^n r(n)^3 (1+6n) \left(\frac{1}{2\sqrt{2}}\right)^{2n} \\ \frac{2}{\pi} &= \sum_{n=0}^{\infty} (-1)^n r(n)^3 (-5+4\sqrt{2}-12n+12\sqrt{2}n) \left(\sqrt{2}-1\right)^{4n} \\ \frac{2}{\pi} &= \sum_{n=0}^{\infty} (-1)^n r(n)^3 (23-10\sqrt{5}+60n-24\sqrt{5}n) \left(\sqrt{5}-2\right)^{4n} \\ \frac{2}{\pi} &= \sum_{n=0}^{\infty} (-1)^n r(n)^3 (177-72\sqrt{6}+420n-168\sqrt{6}n) \left(\sqrt{3}-\sqrt{2}\right)^{8n} \end{aligned}$$

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D. H. Bailey, et. al, *Experimental Mathematics in Action*, A.K. Peters, 2007, pg. 46-49.

## The Wilf-Zeilberger Algorithm for Proving Identities



The Wilf-Zeilberger algorithm is a slick, computer-assisted scheme to prove certain types of sum identities. It provides a nice complement to PSLQ:

- PSLQ permits one to discover new identities, but provides no clue as to how the identities may be rigorously proven.
- The Wilf-Zeilberger scheme permits one to prove certain types of identities, but provides no means to discover the identity.
- Together they make a great combination!

#### Illustrating the Wilf-Zeilberger Method to Prove (1 + 1)<sup>n</sup> = 2<sup>n</sup>

Define

$$F(n,k) = \binom{n}{k} 2^{-n}$$

We wish to show that L(n) = F(n,1) + F(n,2) + ... + F(n,n) = 1 for every n. To that end, use the Wilf-Zeilberger algorithm (implemented in both *Maple* and *Mathematica*) to construct the function

$$G(n,k) = \frac{-1}{2^{n+1}} {n \choose k-1} = \frac{-kF(n,k)}{2(n-k+1)}$$

and observe that

$$F(n+1,k) - F(n,k) = G(n,k+1) - G(n,k)$$

By applying obvious telescoping properties, one can deduce that

$$\sum_{k} F(n+1,k) - \sum_{k} F(n,k) = \sum_{k} (G(n,k+1) - G(n,k)) = 0$$

This establishes that L(n+1) - L(n) = 0 for all n. Since L(0) = 1, we are done.

# An Experimental Math Application of the Wilf-Zeilberger Scheme

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Recall these experimentally-discovered identities:

$$\sum_{n=0}^{\infty} \frac{\binom{4n}{2n} \binom{2n}{n}^4}{2^{16n}} \left(120n^2 + 34n + 3\right) = \frac{32}{n^2}$$
$$\sum_{n=0}^{\infty} \frac{(-1)^n \binom{2n}{n}^5}{2^{20n}} \left(820n^2 + 180n + 13\right) = \frac{128}{\pi^2}$$

Guillera started by defining

$$G(n,k) = \frac{(-1)^k}{2^{16n}2^{4k}} \left(120n^2 + 84nk + 34n + 10k + 3\right) \frac{\binom{2n}{n}^4 \binom{2k}{k}^3 \binom{4n-2k}{2n-k}}{\binom{2n}{k} \binom{n+k}{n}^2}$$

He then used the EKHAD software package to obtain the companion

$$F(n,k) = \frac{(-1)^k 512}{2^{16n} 2^{4k}} \frac{n^3}{4n - 2k - 1} \frac{\binom{2n}{n}^4 \binom{2k}{k}^3 \binom{4n - 2k}{2n - k}}{\binom{2n}{k} \binom{n+k}{n}^2}$$

## **Example Usage of W-Z, Cont.**

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When we define

$$H(n,k) = F(n+1, n+k) + G(n, n+k)$$

Zeilberger's theorem gives the identity

$$\sum_{n=0}^{\infty} G(n,0) = \sum_{n=0}^{\infty} H(n,0)$$

which when written out is

$$\sum_{n=0}^{\infty} \frac{\binom{2n}{n}^4 \binom{4n}{2n}}{2^{16n}} \left( 120n^2 + 34n + 3 \right) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n+7}} \frac{(n+1)^3}{2n+3} \frac{\binom{2n+2}{n+1}^4 \binom{2n}{n}^3 \binom{2n+4}{n+2}}{\binom{2n+2}{n} \binom{2n+1}{2n+1}^2} \\ + \sum_{n=0}^{\infty} \frac{(-1)^n}{2^{20n}} \left( 204n^2 + 44n + 3 \right) \binom{2n}{n}^5 = \frac{1}{4} \sum_{n=0}^{\infty} \frac{(-1)^n \binom{2n}{n}^5}{2^{20n}} \left( 820n^2 + 180n + 13 \right)$$

A limit argument completes the proof of Guillera's identities.

D. H. Bailey, et. al, Experimental Mathematics in Action, A.K. Peters, 2007, pg. 53-55.



The following formulas for zeta(n) have been known for many years:

$$\zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}},$$
  
$$\zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}},$$
  
$$\zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}}.$$

These results have led some to speculate that

$$Q_5 := \zeta(5) / \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}}$$

might be some nice rational or algebraic value.

Sadly, PSLQ calculations have established that if  $Q_5$  satisfies a polynomial with degree at most 25, then at least one coefficient has 380 digits.

#### Apery-Like Relations Found Using Integer Relation Methods

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$$\begin{split} \zeta(5) &= 2\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}} - \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^2}, \\ \zeta(7) &= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} + \frac{25}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \\ \zeta(9) &= \frac{9}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^9 \binom{2k}{k}} - \frac{5}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^2} + 5 \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \\ &+ \frac{45}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^6} - \frac{25}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \sum_{j=1}^{k-1} \frac{1}{j^2}, \\ \zeta(11) &= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^{11} \binom{2k}{k}} + \frac{25}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \\ &- \frac{75}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^8} + \frac{125}{4} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4} \sum_{i=1}^{k-1} \frac{1}{i^4} \end{split}$$

Formulas for 7 and 11 were found by Jonathan Borwein and David Bradley; 5 and 9 are due to Koecher. This general formula was found by Koecher:

$$\sum_{k=1}^{\infty} \frac{1}{k(k^2 - x^2)} = \frac{1}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \frac{5k^2 - x^2}{k^2 - x^2} \prod_{m=1}^{k-1} \left(1 - \frac{x^2}{m^2}\right)$$



Using bootstrapping and an application of the "Pade" function, Borwein and Bradley produced the following remarkable result:

$$\sum_{k=1}^{\infty} \frac{1}{k^3 (1 - x^4/k^4)} = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k} (1 - x^4/k^4)} \prod_{m=1}^{k-1} \left( \frac{1 + 4x^4/m^4}{1 - x^4/m^4} \right)$$

Following an analogous – but more deliberate – experimental-based procedure, DHB, Borwein and Bradley obtained a similar general formula for zeta(2n+2) that is pleasingly parallel to above:

$$\sum_{k=1}^{\infty} \frac{1}{k^2 - x^2} = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k} \left(1 - x^2/k^2\right)} \prod_{m=1}^{k-1} \left(\frac{1 - 4x^2/m^2}{1 - x^2/m^2}\right)$$

Note that this gives an Apery-like formula for zeta(2n), since the LHS equals

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} = \frac{1-\pi x \cot(\pi x)}{2x^2}$$

This experimental discovery will be sketched in the new few slides.



We first conjectured that zeta(2n+2) is a rational combination of terms of the form:

$$\sigma(2r; [2a_1, \cdots, 2a_N]) := \sum_{k=1}^{\infty} \frac{1}{k^{2r} \binom{2k}{k}} \prod_{i=1}^{N} \sum_{n_i=1}^{k-1} \frac{1}{n_i^{2a_i}}$$

where  $r + a_1 + a_2 + ... + a_N = n + 1$  and  $a_i$  are listed in nonincreasing order. We can then write:

$$\sum_{n=0}^{\infty} \zeta(2n+2) x^{2n} \stackrel{?}{=} \sum_{n=0}^{\infty} \sum_{r=1}^{n+1} \sum_{\pi \in \Pi(n+1-r)} \alpha(\pi) \sigma(2r; 2\pi) x^{2n}$$

where  $\Pi(m)$  denotes the additive partitions of m. We can then deduce that

$$\sum_{n=0}^{\infty} \zeta(2n+2) x^{2n} = \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2-x^2)} P_k(x)$$

where  $P_k(x)$  are polynomials whose general form we hope to discover.

## **The Bootstrap Process**



$$\begin{split} \zeta(2) &= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^2} = 3\sigma(2,[0]), \\ \zeta(4) &= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^4} - 9\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1}j^{-2}}{\binom{2k}{k}k^2} = 3\sigma(4,[0]) - 9\sigma(2,[2]) \\ \zeta(6) &= 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}k^6} - 9\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1}j^{-2}}{\binom{2k}{k}k^4} - \frac{45}{2}\sum_{k=1}^{\infty} \frac{\sum_{j=1}^{k-1}j^{-4}}{\binom{2k}{k}k^2} \\ &+ \frac{27}{2}\sum_{k=1}^{\infty}\sum_{j=1}^{k-1} \frac{\sum_{i=1}^{k-1}i^{-2}}{j^2\binom{2k}{k}k^2}, \\ &= 3\sigma(6,[]) - 9\sigma(4,[2]) - \frac{45}{2}\sigma(2,[4]) + \frac{27}{2}\sigma(2,[2,2]) \\ \zeta(8) &= 3\sigma(8,[]) - 9\sigma(6,[2]) - \frac{45}{2}\sigma(4,[4]) + \frac{27}{2}\sigma(4,[2,2]) - 63\sigma(2,[6]) \\ &+ \frac{135}{2}\sigma(2,[4,2]) - \frac{27}{2}\sigma(2,[2,2,2]) \\ \zeta(10) &= 3\sigma(10,[]) - 9\sigma(8,[2]) - \frac{45}{2}\sigma(6,[4]) + \frac{27}{2}\sigma(6,[2,2]) - 63\sigma(4,[6]) \\ &+ \frac{135}{2}\sigma(4,[4,2]) - \frac{27}{2}\sigma(4,[2,2,2]) - \frac{765}{4}\sigma(2,[8]) + 189\sigma(2,[6,2]) \\ &+ \frac{675}{8}\sigma(2,[4,4]) - \frac{405}{4}\sigma(2,[4,2,2]) + \frac{81}{8}\sigma(2,[2,2,2,2]) \end{split}$$

## **Coefficients Obtained**



Partit	Partition Alpha		Partition		Alpha		Partition		Alpha		
[empt	[empty] 3/1		1		-9/1		2		-45/2		
1,1 27/2		27/2	3		-63	/1	2,1		135/2		
1,1,1	1,1,1 -27/2		4	4		5/4	3,1		189/1		
2,2	2,2 675/8		2,1,1		-405/4		1,1,1,1		81/8		
5		-3069/5	4,	4,1		5/4	3,2		945/2		
3,1,1		-567/2	2,	2,2,1		25/8	2,1,1,1		405/4		
1,1,1,	,1,1	-243/40	6	5 -		95/2 5,1			9207/5		
4,2		11475/8	4,	.,1,1 -		85/8	/8 3,3		1323/2		
3,2,1		-2835/2	З,	1,1,1	567	/2	2,2,2		-3375/1	16	
2,2,1,	,1	6075/16	2,	1,1,1,1	-12	15/16	1,1,1,	1, 1, 1	243/80		
7	7 -49149/7		6,	6,1		40/8 5,2			36828/	8	
Partition	Partition Alpha		Partitio		on	Alpha		Partition A		pha	
5,1,1	5,1,1 -27621/10			4,3		32130/8		4,2,1		-3	4425/8
4,1,1,1	4,1,1,1 6885/8			3,3,1		-1587	6/8	3,2,2		-1	4175/8
3,2,1,1		17010/8	3,1,1,1		,1	-1701	/8	2,2,2	,1	10	)125/16
2,2,1,1,1		-6075/16	/16 2,1,1,1		,1,1	729/16		1,1,1,1,1,1,1		-7	29/560
8		-1376235/56		7,1		1179576/56		6,2		85	59950/56
6,1,1 -5		-515970/56		5,3		902286/70		5,2,1		-7	73388/56
5,1,1,1 193347/70			4,4		390150/64		4,3,1		-6	74730/56	
4,2,2 -344250/64		4	4,2,1,1		413100/64		4,1,1,1,1		-4	1310/64	
3,3,2 -277830/56		5	3,3,1,1		166698/56		3,2,2,1		29	)7675/56	
3,2,1,1,1 -119070/56		5	3,1,1,1,1,1		10206/80		2,2,2,2		50	)625/128	
2,2,2,1,1 -60		-60750/64		2,2,1,1	,1,1	18225	64	2,1,1	,1,1,1,1	-1	458/64
1, 1, 1, 1, 1, 1, 1, 1, 1		2187/4480									

#### **Resulting Polynomials**



## After Using "Pade" Function in Mathematica

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$$P_{1}(x) \stackrel{?}{=} 3$$

$$P_{2}(x) \stackrel{?}{=} \frac{3(4x^{2}-1)}{(x^{2}-1)}$$

$$P_{3}(x) \stackrel{?}{=} \frac{12(4x^{2}-1)}{(x^{2}-4)}$$

$$P_{4}(x) \stackrel{?}{=} \frac{12(4x^{2}-1)(4x^{2}-9)}{(x^{2}-4)(x^{2}-9)}$$

$$P_{5}(x) \stackrel{?}{=} \frac{48(4x^{2}-1)(4x^{2}-9)}{(x^{2}-9)(x^{2}-16)}$$

$$P_{6}(x) \stackrel{?}{=} \frac{48(4x^{2}-1)(4x^{2}-9)(4x^{2}-25)}{(x^{2}-9)(x^{2}-16)(x^{2}-25)}$$

$$P_{7}(x) \stackrel{?}{=} \frac{192(4x^{2}-1)(4x^{2}-9)(4x^{2}-25)}{(x^{2}-16)(x^{2}-25)(x^{2}-36)}$$

which immediately suggests the general form:

$$\sum_{n=0}^{\infty} \zeta(2n+2)x^{2n} \stackrel{?}{=} 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2-x^2)} \prod_{m=1}^{k-1} \frac{4x^2-m^2}{x^2-m^2}$$

## **Confirmations of Zeta(2n+2) Formula**



- We symbolically computed the power series coefficients of the LHS and the RHS, and have verified that they agree up to the term with x<sup>100</sup>.
- We verified that Z(1/6), Z(1/2), Z(1/3), Z(1/4), where Z(x) is the RHS, give numerically correct values (analytic values are known for LHS, using the cot formula).
- We then affirmed that the formula gives numerical values with LHS=RHS (to available 400-digit) for 100 pseudorandomly chosen arguments x.
- We subsequently proved this formula two different ways, including using the Wilf-Zeilberger method.

- D. H. Bailey, J. M. Borwein and D. Bradley, "Experimental Determination of Apery-Like Identities for Zeta(2n+2)," 2006, http://crd.lbl.gov/~dhbailey/dhbpapers/apery.pdf.
- D. H. Bailey, et. al, *Experimental Mathematics in Action*, A.K. Peters, 2007, pg. 63-70.

## **History of Numerical Quadrature**



- 1670: Newton devises Newton-Coates integration.
- 1740: Thomas Simpson develops Simpson's rule.
- 1820: Gauss develops Gaussian quadrature.
- 1950-1980: Adaptive quadrature, Romberg integration, Clenshaw-Curtis integration, others.
- 1985-1990: Maple and Mathematica feature built-in numerical quadrature facilities.
- 2000: Very high-precision quadrature (1000+ digits).

With these high-precision values, we can now use PSLQ to obtain analytical evaluations of integrals.

#### The Euler-Maclaurin Formula of Numerical Analysis



$$\int_{a}^{b} f(x) dx = h \sum_{j=0}^{n} f(x_{j}) - \frac{h}{2} (f(a) + f(b))$$
  
- 
$$\sum_{i=1}^{m} \frac{h^{2i} B_{2i}}{(2i)!} \left( f^{(2i-1)}(b) - f^{(2i-1)}(a) \right) - E(h)$$
  
|E(h)|  $\leq 2(b-a) [h/(2\pi)]^{2m+2} \max_{a \leq x \leq b} |D^{2m+2}f(x)|$ 

[Here h = (b - a)/n and  $x_i = a + j h$ . D<sup>m</sup> 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 bellshaped 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.

## Trapezoidal Approximation to a Bell-Shaped Function







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 which the E-M formula applies. Thus 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.



## **Test Integrals**



$$1: \int_{0}^{1} t \log(1+t) dt = 1/4 \qquad 2: \int_{0}^{1} t^{2} \arctan t dt = (\pi - 2 + 2\log 2)/12$$
  

$$3: \int_{0}^{\pi/2} e^{t} \cos t dt = (e^{\pi/2} - 1)/2 \qquad 4: \int_{0}^{1} \frac{\arctan(\sqrt{2+t^{2}})}{(1+t^{2})\sqrt{2+t^{2}}} dt = 5\pi^{2}/96$$
  

$$5: \int_{0}^{1} \sqrt{t} \log t dt = -4/9 \qquad 6: \int_{0}^{1} \sqrt{1-t^{2}} dt = \pi/4$$
  

$$7: \int_{0}^{1} \frac{t}{\sqrt{1-t^{2}}} dt = 1 \qquad 8: \int_{0}^{1} \log t^{2} dt = 2$$
  

$$9: \int_{0}^{\pi/2} \log(\cos t) dt = -\pi \log(2)/2 \qquad 10: \int_{0}^{\pi/2} \sqrt{\tan t} dt = \pi\sqrt{2}/2$$
  

$$11: \int_{0}^{\infty} \frac{1}{1+t^{2}} dt = \pi/2 \qquad 12: \int_{0}^{\infty} \frac{e^{-t}}{\sqrt{t}} dt = \sqrt{\pi}$$
  

$$13: \int_{0}^{\infty} e^{-t^{2}/2} dt = \sqrt{\pi/2} \qquad 14: \int_{0}^{\infty} e^{-t} \cos t dt = 1/2$$

#### Quadratic Convergence with Tanh-Sinh Quadrature



Level	Prob. 1	Prob. 2	Prob. 3	Prob. 4	Prob. 5	Prob. 6	Prob. 7
1	10 <sup>-4</sup>	10 <sup>-4</sup>	$10^{-4}$	10 <sup>-4</sup>	10 <sup>-5</sup>	10 <sup>-5</sup>	$10^{-6}$
2	$10^{-11}$	$10^{-11}$	$10^{-9}$	10 <sup>-9</sup>	10 <sup>-12</sup>	10 <sup>-12</sup>	$10^{-12}$
3	10 <sup>-24</sup>	$10^{-19}$	$10^{-21}$	10 <sup>-18</sup>	10 <sup>-28</sup>	10 <sup>-25</sup>	$10^{-26}$
4	$10^{-51}$	10 <sup>-38</sup>	$10^{-49}$	10 <sup>-36</sup>	10 <sup>-62</sup>	10 <sup>-50</sup>	$10^{-49}$
5	10 <sup>-98</sup>	10 <sup>-74</sup>	$10^{-106}$	10 <sup>-73</sup>	$10^{-129}$	10 <sup>-99</sup>	$10^{-98}$
6	$10^{-195}$	$10^{-147}$	$10^{-225}$	$10^{-145}$	$10^{-265}$	$10^{-196}$	$10^{-194}$
7	10 <sup>-390</sup>	$10^{-293}$	$10^{-471}$	10 <sup>-290</sup>	$10^{-539}$	10 <sup>-391</sup>	$10^{-388}$
8	10 <sup>-777</sup>	$10^{-584}$	$10^{-974}$	10 <sup>-582</sup>		10 <sup>-779</sup>	10 <sup>-777</sup>
Level	Prob. 8	Prob. 9 F	rob. 10	Prob. 11	Prob. 12	Prob. 13	Prob. 14
1	10 <sup>-5</sup>	10-4	10-6	10-2	$10^{-2}$	$10^{-1}$	$10^{-1}$

Levei	Prop. 8	Prop. 9	Prop. 10	Prop. 11	Prop. 12	Prop. 13	Prop. 14
1	$10^{-5}$	$10^{-4}$	10 <sup>-6</sup>	10 <sup>-2</sup>	$10^{-2}$	$10^{-1}$	$10^{-1}$
2	10 <sup>-12</sup>	$10^{-11}$	$10^{-12}$	10 <sup>-5</sup>	10 <sup>-4</sup>	$10^{-3}$	$10^{-2}$
3	10 <sup>-29</sup>	$10^{-24}$	$10^{-25}$	$10^{-11}$	10 <sup>-9</sup>	$10^{-6}$	$10^{-5}$
4	10 <sup>-62</sup>	$10^{-50}$	$10^{-48}$	10 <sup>-22</sup>	$10^{-15}$	$10^{-9}$	$10^{-8}$
5	$10^{-130}$	$10^{-97}$	$10^{-98}$	$10^{-45}$	$10^{-28}$	$10^{-19}$	$10^{-14}$
6	$10^{-266}$	$10^{-195}$	$10^{-194}$	$10^{-91}$	$10^{-50}$	$10^{-37}$	$10^{-26}$
7	$10^{-540}$	$10^{-389}$	$10^{-388}$	$10^{-182}$	$10^{-92}$	$10^{-66}$	$10^{-48}$
8		$10^{-777}$	$10^{-777}$	$10^{-365}$	$10^{-170}$	$10^{-126}$	$10^{-88}$
9				$10^{-731}$	$10^{-315}$	$10^{-240}$	$10^{-164}$
10					$10^{-584}$	$10^{-457}$	$10^{-304}$
11						$10^{-870}$	$10^{-564}$

At level k,  $h = 2^{-k} - i.e.$ , each level halves h and doubles n = # of abscissas.

#### Error Estimation in Tanh-Sinh Quadrature



Let F(t) be the desired integrand function on [a,b]. Define f(t) = F(g(t)) g'(t), where g(t) = tanh (sinh t) (or one of the other g functions above). Then an estimate of the error of the quadrature result, with interval h, is:

$$E_2(h,m) = h(-1)^{m-1} \left(\frac{h}{2\pi}\right)^{2m} \sum_{j=a/h}^{b/h} D^{2m} f(jh)$$

First order (m = 1) estimates are remarkably accurate. Higher-order estimates (m > 1) can be used to obtain "certificates" on the accuracy of a tanh-sinh quadrature result.

This formula was originally discovered due to a "bug" in our computer program – by mistake we implemented this formula and found it to be extremely accurate.

## **Error Estimation Results**



Results for using tanh-sinh quadrature to integrate the function

$$F(t) = 1/(1 + t^2 + t^4 + t^6)$$
 on  $[-1, 1]$ 

h	E(h)	$ E(h) - E_2(h, 1) $
1/1	$5.34967  imes 10^{-3}$	$9.81980  imes 10^{-4}$
1/2	$-3.36641  imes 10^{-4}$	$1.12000  imes 10^{-7}$
1/4	$-3.73280  imes 10^{-8}$	$1.67517  imes 10^{-16}$
1/8	$5.58389  imes 10^{-17}$	$2.29357  imes 10^{-32}$
1/16	$-7.64525  imes 10^{-33}$	$2.07256  imes 10^{-64}$
1/32	$-6.90852  imes 10^{-65}$	$7.23441  imes 10^{-129}$
1/64	$-2.41147  imes 10^{-129}$	$9.08805  imes 10^{-259}$

D. H. Bailey and J. M. Borwein, "Effective Error Estimates in Euler-Maclaurin Based Quadrature Schemes," 2006, http://crd.lbl.gov/~dhbailey/dhbpapers/em-error.pdf.

#### Quadrature and PSLQ: Example 1



Let

$$C(a) = \int_0^1 \frac{\arctan\sqrt{x^2 + a^2}}{(x^2 + 1)\sqrt{x^2 + a^2}} dx$$

Then PSLQ yields

$$C(0) = (\pi \log 2)/8 + G/2$$
  

$$C(1) = \pi/4 - \pi\sqrt{2}/2 + 3\sqrt{2}/2 \cdot \arctan\sqrt{2}$$
  

$$C(\sqrt{2}) = 5\pi^2/96$$

Several general results have now been proven, including

$$\int_{0}^{\infty} \frac{\arctan\sqrt{x^{2} + a^{2}} \, dx}{(x^{2} + 1)\sqrt{x^{2} + a^{2}}} = \frac{\pi}{2\sqrt{a^{2} - 1}} \left(2 \arctan\sqrt{a^{2} - 1} - \arctan\sqrt{a^{4} - 1}\right)$$



$$\frac{2}{\sqrt{3}} \int_{0}^{1} \frac{\log^{6} x \arctan[x\sqrt{3}/(x-2)]}{x+1} dx = \frac{1}{81648} \left(-229635L_{3}(8) + 29852550L_{3}(7)\log 3\right) \\ -1632960L_{3}(6)\pi^{2} + 27760320L_{3}(5)\zeta(3) \\ -275184L_{3}(4)\pi^{4} + 36288000L_{3}(3)\zeta(5) \\ -30008L_{3}(2)\pi^{6} - 57030120L_{3}(1)\zeta(7)\right)$$

where

$$L_{-3}(s) = \sum_{n=1}^{\infty} \left[ \frac{1}{(3n-2)^s} - \frac{1}{(3n-1)^s} \right]$$

is the Dirichlet series. Numerous other results have been found.

D. H. Bailey, et. al, *Experimental Mathematics in Action*, A.K. Peters, 2007, pg. 43,44,61.

#### A Log-Tan Integral Identity from Mathematical Physics



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

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.





#### Define

$$J_n = \int_{n\pi/60}^{(n+1)\pi/60} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt$$

Then

$$0 \stackrel{?}{=} -2J_2 - 2J_3 - 2J_4 + 2J_{10} + 2J_{11} + 3J_{12} + 3J_{13} + J_{14} - J_{15} - J_{16} - J_{17} - J_{18} - J_{19} + J_{20} + J_{21} - J_{22} - J_{23} + 2J_{25}$$

This has been verified to over 1000 digits. The interval for  $J_{23}$  is the interval that includes the singularity.

### 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**<sub>n</sub>



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:

$$C_{1} = 2$$
  

$$C_{2} = 1$$
  

$$C_{3} = L_{-3}(2) = \sum_{n \ge 0} \left( \frac{1}{(3n+1)^{2}} - \frac{1}{(3n+2)^{2}} \right)$$
  

$$C_{4} = 14\zeta(3)$$

Limiting Value of C<sub>n</sub>



The C<sub>n</sub> numerical values approach a limit:

- $C_{10} = 0.6318800241470122229035087366080283...$
- $C_{40} = 0.63047350337836353186994190185909694...$
- $C_{100} = 0.63047350337438679612204019271903171...$
- $C_{200} = 0.63047350337438679612204019271087890...$

What is this limit? 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**



 $D_2 = 1/3$  $D_3 = 8 + 4\pi^2/3 - 27 L_{-3}(2)$  $D_4 = 4\pi^2/9 - 1/6 - 7\zeta(3)/2$  $E_2 = 6 - 8 \log 2$  $E_3 = 10 - 2\pi^2 - 8 \log 2 + 32 \log^2 2$  $E_4 = 22 - 82\zeta(3) - 24 \log 2 + 176 \log^2 2 - 256(\log^3 2)/3$  $+16\pi^2 \log 2 - 22\pi^2/3$  $E_5 \stackrel{\prime}{=} 42 - 1984 \operatorname{Li}_4(1/2) + 189\pi^4/10 - 74\zeta(3) - 1272\zeta(3) \log 2$  $+40\pi^{2}\log^{2} 2 - 62\pi^{2}/3 + 40(\pi^{2}\log 2)/3 + 88\log^{4} 2$  $+464 \log^2 2 - 40 \log 2$ 

## The Ising Integral E<sub>5</sub>



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 highprecision 3-D quadrature program. Then we used PSLQ to discover the evaluation given on the previous page.

 $E_{5} = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-y)^{2}(1-xy)^{2}(1-z)^{2}(1-yz)^{2}(1-xyz)^{2} \left( -\left[ 4(x+1)(xy+1)\log(2)\left(y^{5}z^{3}x^{7}-y^{4}z^{2}(4(y+1)z+3)x^{6}-y^{3}z\left((y^{2}+1\right)z^{2}+4(y+1)z^{2}\right) \right] \right] dx + \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-xy)^{2}(1-xy)^{2}(1-xyz)^{2}(1-xyz)^{2} \left( -\left[ 4(x+1)(xy+1)\log(2)\left(y^{5}z^{3}x^{7}-y^{4}z^{2}(4(y+1)z+3)x^{6}-y^{3}z\left((y^{2}+1\right)z^{2}+4(y+1)z^{2}\right) \right] \right] dx + \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-xy)^{2}(1-xy)^{2}(1-xyz)^{2}(1-xyz)^{2} \left( -\left[ 4(x+1)(xy+1)\log(2)\left(y^{5}z^{3}x^{7}-y^{4}z^{2}(4(y+1)z+3)x^{6}-y^{3}z\left((y^{2}+1\right)z^{2}+4(y+1)z^{2}\right) \right] \right] dx + \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-xy)^{2}(1-xy)^{2}(1-xyz)^{2}(1-xyz)^{2} \left( -\left[ 4(x+1)(xy+1)\log(2)\left(y^{5}z^{3}x^{7}-y^{4}z^{2}\right) \right] \right] \right] dx + \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-xy)^{2}(1-xy)^{2}(1-xyz)^{2} \left( -\left[ 4(x+1)(xy+1)\log(2)\left(y^{5}z^{3}x^{7}-y^{4}z^{2}\right) \right] \right] dx + \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-xy)^{2}(1-xy)^{2}(1-xy)^{2}(1-xy)^{2} \right] dx + \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \left[ 2(1-x)^{2}(1-xy)^{2}($  $1)z + 5)x^{5} + y^{2} (4y(y + 1)z^{3} + 3(y^{2} + 1)z^{2} + 4(y + 1)z - 1)x^{4} + y(z(z^{2} + 4z + 5)y^{2} + 4(z^{2} + 1)y + 5z + 4)x^{3} + ((-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} - 4zy + 1)x^{2} + (-3z^{2} - 4z + 1)y^{2} +$  $-(y(5z+4)+4)x-1)]/[(x-1)^{3}(xy-1)^{3}(xyz-1)^{3}] + [3(y-1)^{2}y^{4}(z-1)^{2}z^{2}(yz-1)^{2}x^{6}+2y^{3}z(3(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}y^{5}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}+z^{2}(5z^{3}+3z^{2}+3z+5)y^{4}+(z-1)^{2}z^{3}+z^{2}+z$  $(5z^{2} + 16z + 5)y^{3} + (3z^{5} + 3z^{4} - 22z^{3} - 22z^{2} + 3z + 3)y^{2} + 3(-2z^{4} + z^{3} + 2z^{2} + z - 2)y + 3z^{3} + 5z^{2} + 5z + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2} + 5z^{2} + 5z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2} + 5z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 5z^{2} + 5z^{2} + 3)x^{5} + y^{2}(7(z - 1)^{2}z^{4}y^{6} - 2z^{3}(z^{3} + 15z^{2})y^{2} + 3z^{3} + 3z^{3} + 5z^{2} + 5z^{3} + 3z^{3} + 3z^$  $+15z + 1)y^{5} + 2z^{2} \left(-21z^{4} + 6z^{3} + 14z^{2} + 6z - 21\right)y^{4} - 2z \left(z^{5} - 6z^{4} - 27z^{3} - 27z^{2} - 6z + 1\right)y^{3} + \left(7z^{6} - 30z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{3} + 28z^{2} - 30z + 7\right)y^{2} - 2 \left(7z^{5} + 28z^{4} + 54z^{2} + 54z^{2} + 28z^{2} + 28z^{2} + 28z^{2} + 28z^{2} + 28z^{2} + 30z^{2} + 28z^{2} + 28$  $+15z^{4} - 6z^{3} - 6z^{2} + 15z + 7)y + 7z^{4} - 2z^{3} - 42z^{2} - 2z + 7)x^{4} - 2y(z^{3}(z^{3} - 9z^{2} - 9z + 1)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{5} + z(7z^{5} + 14z^{4} + 3)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{5} + z(7z^{5} + 14z^{4} + 3)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{3} - 18z^{2} - 14z + 7)y^{6} + z^{2}(7z^{4} - 14z^{4} - 14z^{4}$  $z^{3} + 3z^{2} + 14z + 7)y^{4} + (z^{6} - 14z^{5} + 3z^{4} + 84z^{3} + 3z^{2} - 14z + 1)y^{3} - 3(3z^{5} + 6z^{4} - z^{3} - z^{2} + 6z + 3)y^{2} - (9z^{4} + 14z^{3} - 14z^{2} + 14z + 9)y + z^{3} + 7z^{2} + 7z$  $+1)x^{3} + \left(z^{2}\left(11z^{4} + 6z^{3} - 66z^{2} + 6z + 11\right)y^{6} + 2z\left(5z^{5} + 13z^{4} - 2z^{3} - 2z^{2} + 13z + 5\right)y^{5} + \left(11z^{6} + 26z^{5} + 44z^{4} - 66z^{3} + 44z^{2} + 26z + 11\right)y^{4} + \left(6z^{5} - 4z^{4} + 22z^{4} +$  $+5z^{3} - 22z^{2} + 5z + 22)y^{4} + (5z^{5} + 5z^{4} - 26z^{3} - 26z^{2} + 5z + 5)y^{3} + (3z^{4} - 22z^{3} - 26z^{2} - 22z + 3)y^{2} + (3z^{3} + 5z^{2} + 5z + 3)y + 5z^{2} + 22z + 5)x + 15z^{2} + 2z$  $+2y(z-1)^{2}(z+1)+2y^{3}(z-1)^{2}z(z+1)+y^{4}z^{2}(15z^{2}+2z+15)+y^{2}(15z^{4}-2z^{3}-90z^{2}-2z+15)+15]/[(x-1)^{2}(y-1)^{2}(xy-1)^{2}(xy-1)^{2}(yz-1)^{2$  $(xyz-1)^{2}\left] - \left[4(x+1)(y+1)(yz+1)\left(-z^{2}y^{4}+4z(z+1)y^{3}+\left(z^{2}+1\right)y^{2}-4(z+1)y+4x\left(y^{2}-1\right)\left(y^{2}z^{2}-1\right)+x^{2}\left(z^{2}y^{4}-4z(z+1)y^{3}-\left(z^{2}+1\right)y^{2}-4(z+1)y^{2}+2z^{2}+1\right)y^{2}-4(z+1)y^{2}+2z^{2}+1\right)\right] + 2z^{2}y^{4} + 2z^{2}y^{4} + 2z^{2}y^{4} + 2z^{2}y^{4} + 2z^{2}y^{4} + 2z^{2}+1\right)y^{2} + 2z^{2}y^{4} + 2z^{2}+1\right)y^{2} + 2z^{2}y^{4} + 2z^{2}y^{4} + 2z^{2}+1\right)y^{2} + 2z^{2}y^{4} + 2z^{2}+1\right)y^{2} + 2z^{2}+1\right)y^{2} + 2z^{2}+1$  $+4(z+1)y+1)-1)\log(x+1)]/[(x-1)^{3}x(y-1)^{3}(yz-1)^{3}] - [4(y+1)(xy+1)(z+1)(x^{2}(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{3}-(x^{2}+1)(z^{2}-4z-1)y^{4}+4x(x+1)(z^{2}-1)y^{4}+4x(x+1$  $y^{2} - 4(x+1)(z^{2}-1)y + z^{2} - 4z - 1)\log(xy+1)] / [x(y-1)^{3}y(xy-1)^{3}(z-1)^{3}] - [4(z+1)(yz+1)(x^{3}y^{5}z^{7} + x^{2}y^{4}(4x(y+1)+5)z^{6} - xy^{3}((y^{2}+1)^{3}y^{6}z^{7} + x^{2}y^{6}) + x^{2}(y^{2}+1)^{3}(y^{2}+1)^{$  $1) x^{2} - 4(y+1)x - 3) z^{5} - y^{2} (4y(y+1)x^{3} + 5(y^{2}+1)x^{2} + 4(y+1)x + 1) z^{4} + y(y^{2}x^{3} - 4y(y+1)x^{2} - 3(y^{2}+1)x - 4(y+1)) z^{3} + (5x^{2}y^{2} + y^{2} + 4x(y+1)x^{2} - 3(y^{2}+1)x^{2} - 3(y^{2}+1)x^{2}$  $y+1)z^{2} + \left((3x+4)y+4)z-1\right)\log(xyz+1)\right] / \left[xy(z-1)^{3}z(yz-1)^{3}(xyz-1)^{3}\right] \right) \left] / \left[(x+1)^{2}(y+1)^{2}(xy+1)^{2}(z+1)^{2}(yz+1)^{2}(xyz+1)^{2}\right] + \left[(x+1)^{2}(xy+1)^{2}$ dx dy dz



Consider the 2-parameter class of Ising integrals

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

(odd k has a direct connection to QFT). 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:

$$0 = C_{3,0} - 84C_{3,2} + 216C_{3,4}$$

$$0 = 2C_{3,1} - 69C_{3,3} + 135C_{3,5}$$

$$0 = C_{3,2} - 24C_{3,4} + 40C_{3,6}$$

$$0 = 32C_{3,3} - 630C_{3,5} + 945C_{3,7}$$

$$0 = 125C_{3,4} - 2172C_{3,6} + 3024C_{3,8}$$

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*, to appear, http://crd.lbl.gov/~dhbailey/dhbpapers/meijer/pdf.



## **Experimental Recursion for n = 24**

 $0 \stackrel{?}{=} C_{24,1}$ 

-1107296298*C*<sub>24,3</sub>

 $+1288574336175660C_{24,5}$ 

 $-88962910652291256000 C_{24,7}$ 

 $+1211528914846561331193600 C_{24,9}$ 

 $-5367185923241422152980553600\,C_{\mathbf{24},11}$ 

 $+9857686103738772925980190636800C_{24,13}$ 

 $-8476778037073141951236532459008000C_{24,15}$ 

 $+3590120926882411593645052529049600000C_{24,17}$ 

 $-745759114781380983188217871663104000000C_{24,19}$ 

 $+71215552121869985477578381170258739200000C_{24,21}$ 

 $-2649853457247995406113355087174696960000000C_{24,23}$ 

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

Jonathan M. Borwein and Bruno Salvy, "A Proof of a Recursion for Bessel Moments," manuscript, 2007, http://users.cs.dal.ca/~jborwein/recursion.pdf.



where  $c_{n,k} = n! k! 2^{-n} C_{n,k}$ , where K(y) is the complete elliptic integral function, and

$$y = \sqrt{\frac{(1-3x)(1+x)^3}{(1+3x)(1-x)^3}}$$

## **Cautionary Example**



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

$$\int_{0}^{\infty} \cos(2x) \prod_{n=0}^{\infty} \cos(x/n) dx =$$
0.39269908169872415480783042290993786052464543418723...
$$\frac{\pi}{8} =$$
0.39269908169872415480783042290993786052464617492189...

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



- Advanced techniques for computing high-precision definite integrals, infinite series, etc., combined with the PSLQ algorithm, have yielded hundreds of new results of mathematics and mathematical physics.
- These methods typically do not suggest proofs, but often it is much easier to find a proof when one "knows" the answer is right.

Questions:

- Can we better understand the theoretical underpinnings of these computational methods?
- Can we develop better methods for tasks such as infinite series summation and multi-dimensional quadrature?
- Can we adapt these methods to extremely highly parallel computer systems?
- Can we better incorporate advanced developments in computer science multi-core processors, advanced visualization, database management, compiler and language tools, etc?
- How can we train students in experimental math?