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Effective Error Bounds for Euler-MacLaurin based Numerical Quadrature

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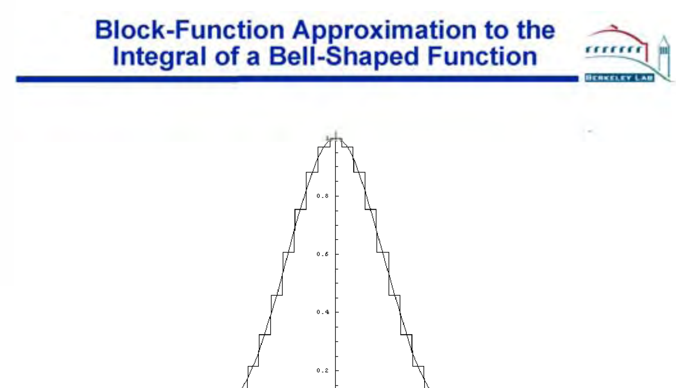
Canada Research Chair in Collaborative Technology

hpcs 2006

Joint work with David Bailey, Lawrence Berkeley

The purpose of computing is insight not numbers
(Richard Hamming 1962)



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Revised 16/04/06

ABSTRACT

► We analyze the behavior of Euler-Maclaurin-based integration schemes with the intention of deriving accurate and economic estimations of the error

► These schemes typically provide very high-precision results (hundreds or thousands of digits), in reasonable run time, even when the integrand function has a blow-up singularity or infinite derivative at an endpoint

►Heretofore, researchers using these schemes have relied mostly on ***ad hoc*** error estimation schemes to project the estimated error of the present iteration

►In this paper, we seek to develop some more rigorous, yet highly usable schemes to estimate these errors

INTRODUCTION

► In the past few years, computation of definite integrals to high precision has become a key tool in **experimental math.**

- ►It is often possible to recognize an unknown definite integral if its numerical value is known to extremely high precision

►High precision is required since *integer relation searches* of n terms with d-digit coefficients require at least dn-digit precision for both input data and relation searching.

- ►Such computation often requires *highly parallel implementation*

►One computation below, required nearly one hour on 1024 cpus, and the PSLQ integer relation search in another required 44 hours on 32 cpus. Moreover, such extreme computations provide excellent tests of HPC systems

- ► for example, we identified a difficulty with differing processor speeds on the Virginia Tech system with these calculations

OUTLINE

- ► **Experimental Mathematics**
  - ► Rationale
  - ► Examples of need for quadrature etc

- ► **Extreme Quadrature**
  - ► Theory
  - ► Implementation
  - ► Examples

Dalhousie Distributed Research Institute and Virtual Environment

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Fully Interactive multi-way audio and visual

Given good bandwidth audio is much harder

The closest thing to being in the same room

Shared Desktop for viewing presentations or sharing software

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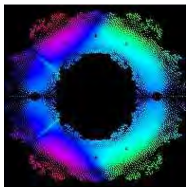

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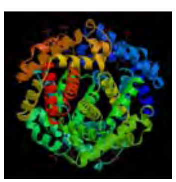

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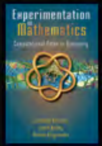

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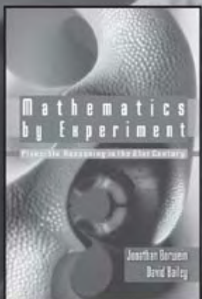

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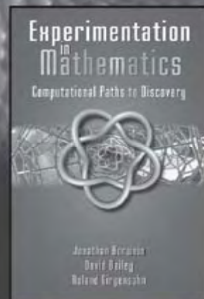

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short time since the first editions of *Mathematics by Experiment: Plausible Reaso*
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Specific case studies include:
-- analytic evaluation of integrals by means of symbolic and numeric computing techniques
-- evaluation of Apery-like summations
-- finding dependencies among high-dimension vectors (with applications to factoring large integers)
-- inverse scattering (reconstruction of physical objects based on electromagnetic or acoustic scattering)
-- investigation of continuous but nowhere differentiable functions.

In addition to these case studies, the book includes some background on the computational techniques used in these analyses.

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Mathematics by Experiment: Plausible Reasoning in the 21st Century

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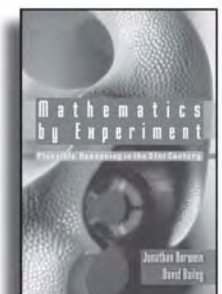

". . . experimental mathematics is here to stay. The reader who wants to get an introduction to this exciting approach to doing mathematics can do no better than [this book]."

— *Notices* of the AMS

ISBN 1-56881-211-6; Hardcover; 298 pp.; $45.00

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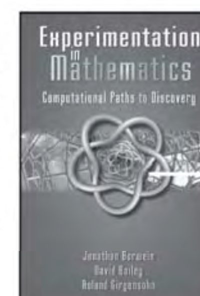

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MATH LAB

Computer experiments are transforming mathematics

BY ERICA KLARREICH

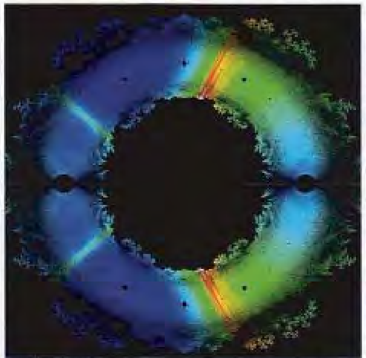
Science News 2004

Many people regard mathematics as the crown jewel of the sciences. Yet math has historically lacked one of the defining trappings of science: laboratory equipment. Physicists have their particle accelerators; biologists, their electron microscopes; and astronomers, their telescopes. Mathematics, by contrast, concerns not the physical landscape but an idealized, abstract world. For exploring that world, mathematicians have traditionally had only their intuition.

Now, computers are starting to give mathematicians the lab instrument that they have been missing. Sophisticated software is enabling researchers to travel further and deeper into the mathematical universe. They're calculating the number pi with mind-boggling precision, for instance, or discovering patterns in the contours of beautiful, infinite chains of spheres that arise out of the geometry of knots.

Experiments in the computer lab are leading mathematicians to discoveries and insights that they might never have reached by traditional means. "Pretty much every [mathematical] field has been transformed by it," says Richard Crandall, a mathematician at Reed College in Portland, Ore. "Instead of just being a number-crunching tool, the computer is becoming more like a garden shovel that turns over rocks, and you find things underneath."

At the same time, the new work is raising unsettling questions about how to regard experimental results



UNSOLVED MYSTERIES — A computer experiment produced this plot of all the solutions to a collection of simple equations in 2001. Mathematicians are still trying to account for its many features.

"I have some of the excitement that Leonardo of Pisa must have felt when he encountered Arabic arithmetic. It suddenly made certain calculations flabbergastingly easy," Borwein says. "That's what I think is happening with computer experimentation today."

EXPERIMENTERS OF OLD In one sense, math experiments are nothing new. Despite their field's reputation as a purely deductive science, the great mathematicians over the centuries have never limited themselves to formal reasoning and proof.

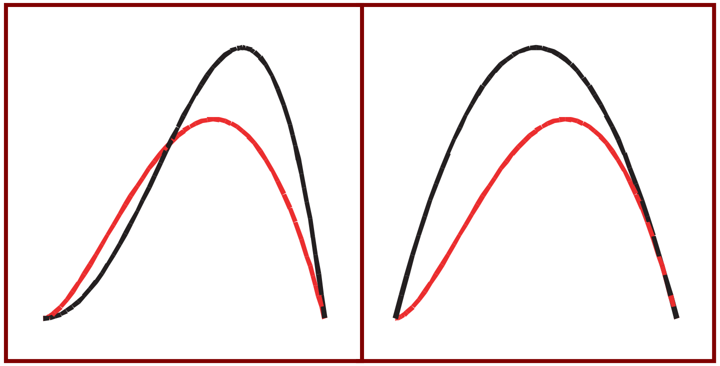
For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

Carl Friedrich Gauss, one of the towering figures of 19th-century mathematics, habitually discovered new mathematical results by experimenting with numbers and looking for patterns. When Gauss was a teenager, for instance, his experiments led him to one of the most important conjectures in the history of number theory: that the number of prime numbers less than a number x is roughly equal to x divided by the logarithm of x.

Gauss often discovered results experimentally long before he could prove them formally. Once, he complained, "I have the result, but I do not yet know how to get it."

In the case of the prime number theorem, Gauss later refined his conjecture but never did figure out how to prove it. It took more than a century for mathematicians to come up with a proof.

Like today's mathematicians, math experimenters in the late 19th century used computers—but in those days, the word referred to people with a special facility for calcu-



Comparing $-y^2\ln(y)$ (red) to $y-y^2$ and y^2-y^4

WARMUP Computational Proof

Suppose we know that 1<N<10 and that N is an integer

- **computing N to 1 significant place** with a certificate will prove the value of N. *Euclid's method* is basic to such ideas.

Likewise, suppose we know α is *algebraic of degree d and length λ*

(coefficient sum in absolute value)

If P is polynomial of degree D & length L **EITHER** $P(\alpha) = 0$ **OR**

$$|P(\alpha)| \geq \frac{1}{L^{d-1}\lambda^{D}}$$

Example (MAA, April 2005). Prove that

$$\int_{-\infty}^{\infty} \frac{y^2}{1+4\,y+y^6-2\,y^4-4\,y^3+2\,y^5+3\,y^2}\,dy = \pi$$

Proof. Purely **qualitative analysis** with partial fractions and arctans shows the integral is $\pi\ \beta$ where β is algebraic of degree *much* less than **100 (actually 6)**, length *much* less than **100,000,000**.With **P(x)=x-1** (D=1,L=2, d=6, λ=?), this means *checking* the identity to **100** places is plenty of **PROOF.**

A fully symbolic Maple proof followed. **QED**

$$|\beta - 1| < 1/(32\lambda) \mapsto \beta = 1$$

Ising Integrals (Jan 2006)

The following integrals arise in Ising theory of mathematical physics:

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

Richard Crandall showed that this can be transformed to a 1-D integral:

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

where K_0 is a modified Bessel function. We then computed 400-digit numerical values, from which these results were found (and proven):

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

$$C_4 = 14\zeta(3)$$

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

- via **PSLQ** and the **Inverse Calculator** to which we now turn

Fast Arithmetic
(Complexity Reduction in Action)

Multiplication

- Karatsuba multiplication (200 digits +) or Fast Fourier Transform (FFT)

… in ranges from 100 to 1,000,000,000,000 digits

- The other operations $\times, \div, \sqrt{\cdot}$
  via Newton's method
- Elementary and special functions
  via Elliptic integrals and Gauss AGM

$$O\left(n^{\log_2(3)}\right)$$

For example:

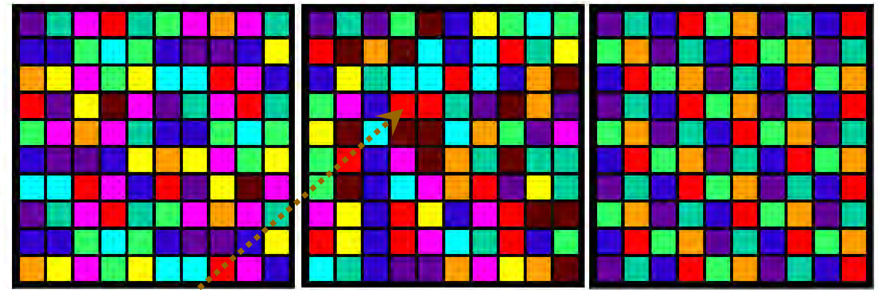
$$\begin{aligned}&\left(a+c\cdot 10^N\right)\times\left(b+d\cdot 10^N\right)\\ =\;& ab+(ad+bc)\cdot 10^N+cd\cdot 10^{2N}\\ =\;& ab+\underbrace{\{(a+c)(b+d)-ab-cd\}}_{\text{three multiplications}}\cdot 10^N+cd\cdot 10^{2N}\end{aligned}$$

Karatsuba replaces one 'times' by many 'plus'

FFT multiplication of multi-billion digit numbers reduces centuries to minutes. Trillions must be done with Karatsuba!

A Colour and an Inverse Calculator (1995)

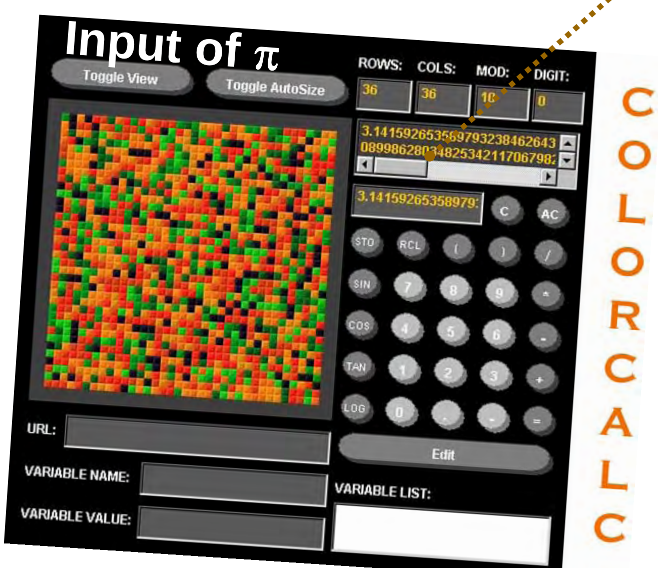
Inverse Symbolic Computation



Archimedes: $223/71 < \pi < 22/7$

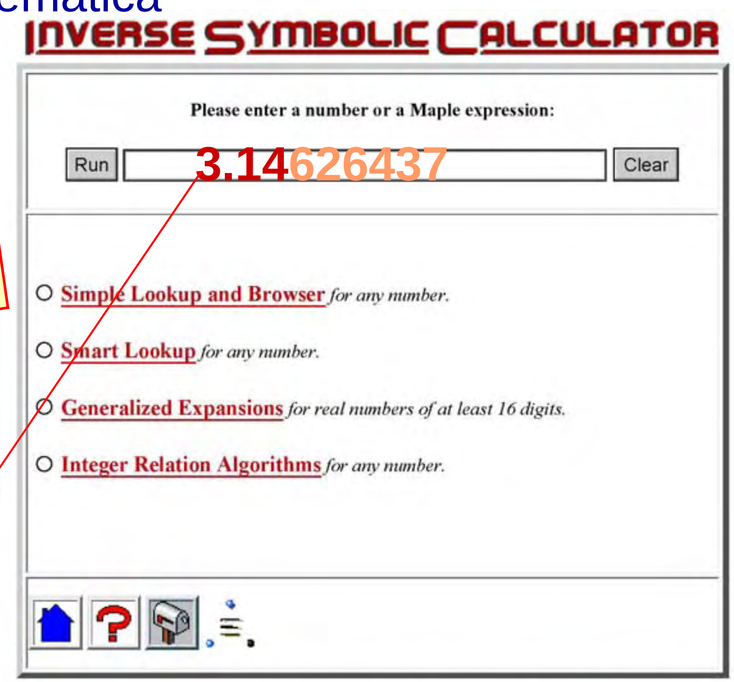
Inferring mathematical structure from numerical data

- Mixes *large table lookup*, integer relation methods and intelligent preprocessing – needs ***micro-parallelism***
- It faces the “curse of exponentiality”
- Implemented as **Recognize** in Mathematica and **identify** in Maple



identify(sqrt(2.)+sqrt(3.))

$$\sqrt{2} + \sqrt{3}$$



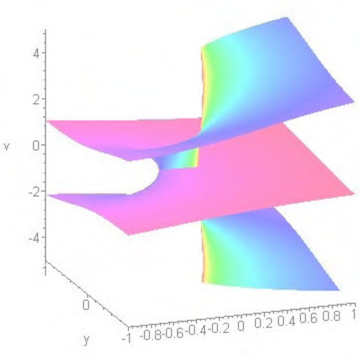
Expressions that are **not** numeric like ln(Pi*sqrt(2)) are evaluated in Maple in symbolic form first, followed by a floating point evaluation followed by a lookup.

Knuth's Problem

A guided proof followed on **asking why** Maple could compute the answer so fast.

The answer is Gonnet's **Lambert's W** which solves

W exp(W) = x

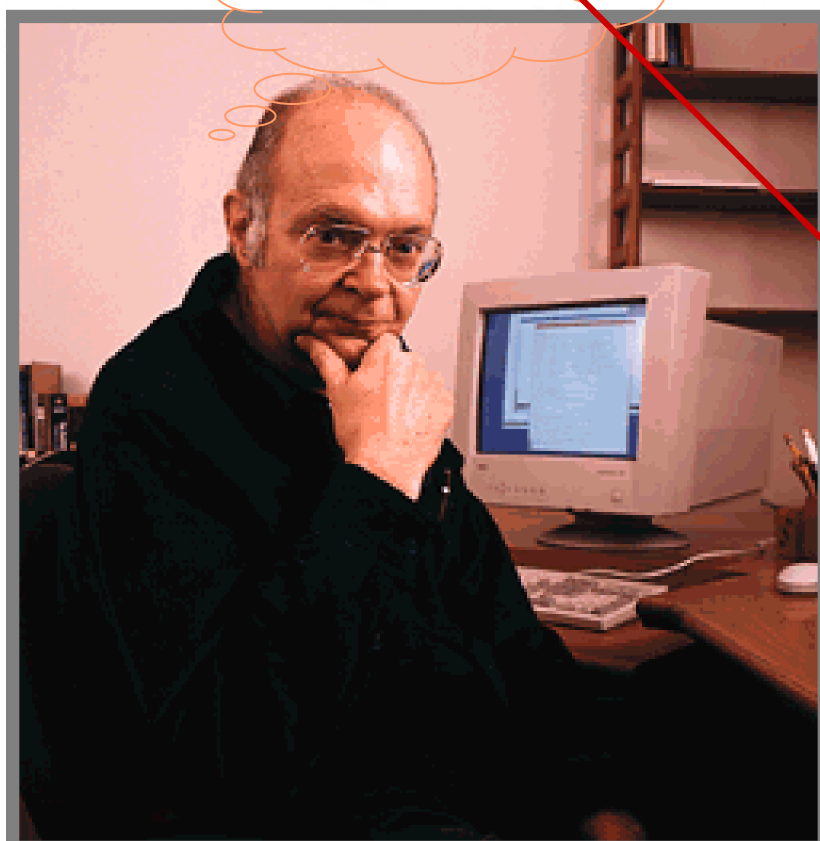


W's **Riemann** surface

Donald Knuth* asked for a closed form evaluation of:

$$\sum_{k=1}^{\infty}\left\{\frac{k^k}{k!\,e^k}-\frac{1}{\sqrt{2\pi k}}\right\} = -0.084069508727655\ldots.$$

"instrumentation"



te 20 or 200 digits

shown on next slide

in the *Inverse Sym-*

turns

$$\approx \frac{2}{3}+\frac{\zeta(1/2)}{\sqrt{2\pi}}.$$

ich *Maple* 9.5 on a

in under 6 seconds

*** ARGUABLY WE ARE DONE**

ENTERING

evalf(Sum(k^k/k!/exp(k)-1/sqrt(2*Pi*k),k=1..infinity),16)

'Simple Lookup' fails;
'Smart Look up' gives:

INVERSE SYMBOLIC CALCULATOR

The ISC is the **Inverse Symbolic Calculator**, a set of programs and specialized tables of mathematical constants dedicated to the identification of real numbers. It also serves as a way to produce identities with functions and real numbers. It is one of the main ongoing projects at the Centre for Experimental and Constructive Mathematics (CECM).

Results of the search:

Maple output:

.08406950872765600

.8406950872765600e-1

Value to be looked up: .8406950872765600e-1 = K

Performing a smart lookup on .8406950872765600e-1:

Function	Result	Precision	Matches
K-2/3	.5825971579390106666666666	16	1

579390106 was probably generated by one
s or found in one of the given tables.
Answers are given from shortest to longest description

Mixed constants with 5 operations

5825971579390106 = Zeta(1/2)/sr(2)/sr(Pi)

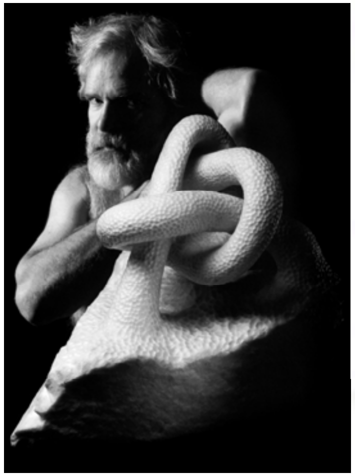
Browse around .5825971579390106.

Integer Relation Methods

The PSLQ Integer Relation Algorithm

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

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

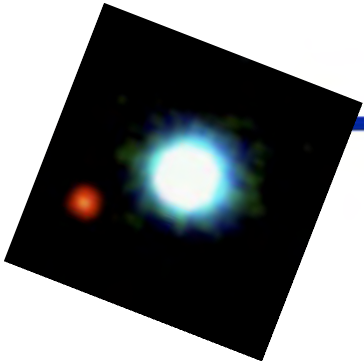


- At the present time, the PSLQ algorithm of mathematician-sculptor Helaman Ferguson is the best-known integer relation algorithm.
- PSLQ was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.
- High precision arithmetic software is required: at least d x n digits,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

An Immediate Use

To see if a is algebraic of degree N, consider $(1,a,a^2,\ldots,a^N)$

Combinatorial optimization for pure mathematics (also LLL)



Application of PSLQ: Bifurcation Points in Chaos Theory

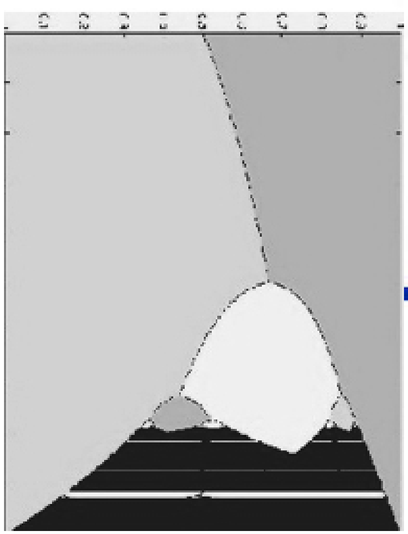
B_3 = 3.54409035955… is third bifurcation point of the logistic iteration of chaos theory:

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

i.e., B_3 is the smallest r such that the iteration exhibits 8-way periodicity instead of 4-way periodicity.

In 1990, a predecessor to PSLQ found that B_3 is a root of the polynomial

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



Recently B_4 was identified as the root of a 256-degree polynomial by a much more challenging computation.

These results have subsequently been proven formally.

- The proofs use **Groebner basis** techniques
- Another useful part of the HPM toolkit

PSLQ and Zeta

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$$

Euler (1707-73)

$$= \frac{\pi^2}{6}, \zeta(4) = \frac{\pi^4}{90}, \zeta(6) = \frac{\pi^6}{945}, \cdots$$

1. via PSLQ to 50,000 digits (250 terms)

2005 Bailey, Bradley & JMB *discovered and proved* - in Maple - three *equivalent* binomial identities

$$\mathcal{Z}(x) = 3\sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k}(k^2-x^2)} \prod_{n=1}^{k-1} \frac{4x^2-n^2}{x^2-n^2}$$

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

$$= \frac{1-\pi x \cot(\pi x)}{2x^2}$$

1

2. reduced as hoped

2

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

3

$$_3F_2\left(\begin{matrix} 3n, n+1, -n \\ 2n+1, n+1/2 \end{matrix}; \frac{1}{4}\right) = \frac{\binom{2n}{n}}{\binom{3n}{n}}$$

3. was easily **computer proven** (Wilf-Zeilberger)
MAA: human proof?

hpcs 2006

Extreme Quadrature.
Ising Susceptibility Integrals

Bailey, Crandall and I are currently studying:

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

The first few values are known: $D_1=2$, $D_2=2/3$, while

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

and

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

- ✓ Computer Algebra Systems can (with help) find the first 3
- ✓ **D_4 is a remarkable 1977 result due to McCoy--Tracy--Wu**

TANH-SINH QUADRATURE

► is the fastest known high-precision scheme, particularly if one counts time for computing abscissas and weights

- ► has been successfully used for quadrature calculations up to 20,000-digit precision
- ► works well for functions with blow-up singularities or infinite derivatives at endpoints, and is well-suited for highly parallel implementation

►At present, these schemes rely on ad-hoc methods to estimate the error at any given stage

- ► one can simply continue until two iterations give the same result (except for the last few digits)
- ►but this nearly doubles overall run time, which is an issue for large quadrature computations attempted on highly parallel computers

►Also, while one can readily compute very high-precision values with these methods, mathematicians often require “certificates”

- ► rigorous guarantees that the approximation error cannot exceed a given level

►Hence we seek much more accurate and rigorous, yet readily computable error bounds for this class of quadrature methods

Quadrature and the Euler-Maclaurin Formula

Atkinson's version of the Euler-Maclaurin formula. For m > 0 integer, assume h evenly divides a and b, while f(x) is at least (2 m +2)-times continuously differentiable on [a, b]. Then

$$\int_a^b f(x)\,dx \;=\; h\sum_{j=a/h}^{b/h} f(jh) - \frac{h}{2}[f(a)+f(b)]$$
$$-\sum_{i=1}^{m}\frac{h^{2i}B_{2i}}{(2i)!}\left[D^{2i-1}f(b)-D^{2i-1}f(a)\right]+E(h,m),$$

where B_j denotes the j-th Bernoulli number, D denotes the differentiation operator, and the **error** is

$$E(h,m) \;=\; \frac{(a-b)\,B_{2m+2}\,D^{2m+2}f(\xi)}{(2m+2)!}\,h^{2m+2},$$

where $\xi \in$ (a, b).

► Suppose f(t) and all derivatives are zero at the endpoints (as for a smooth, bell-shaped function). Then the 2nd and 3rd terms of the E-M formula are zero.

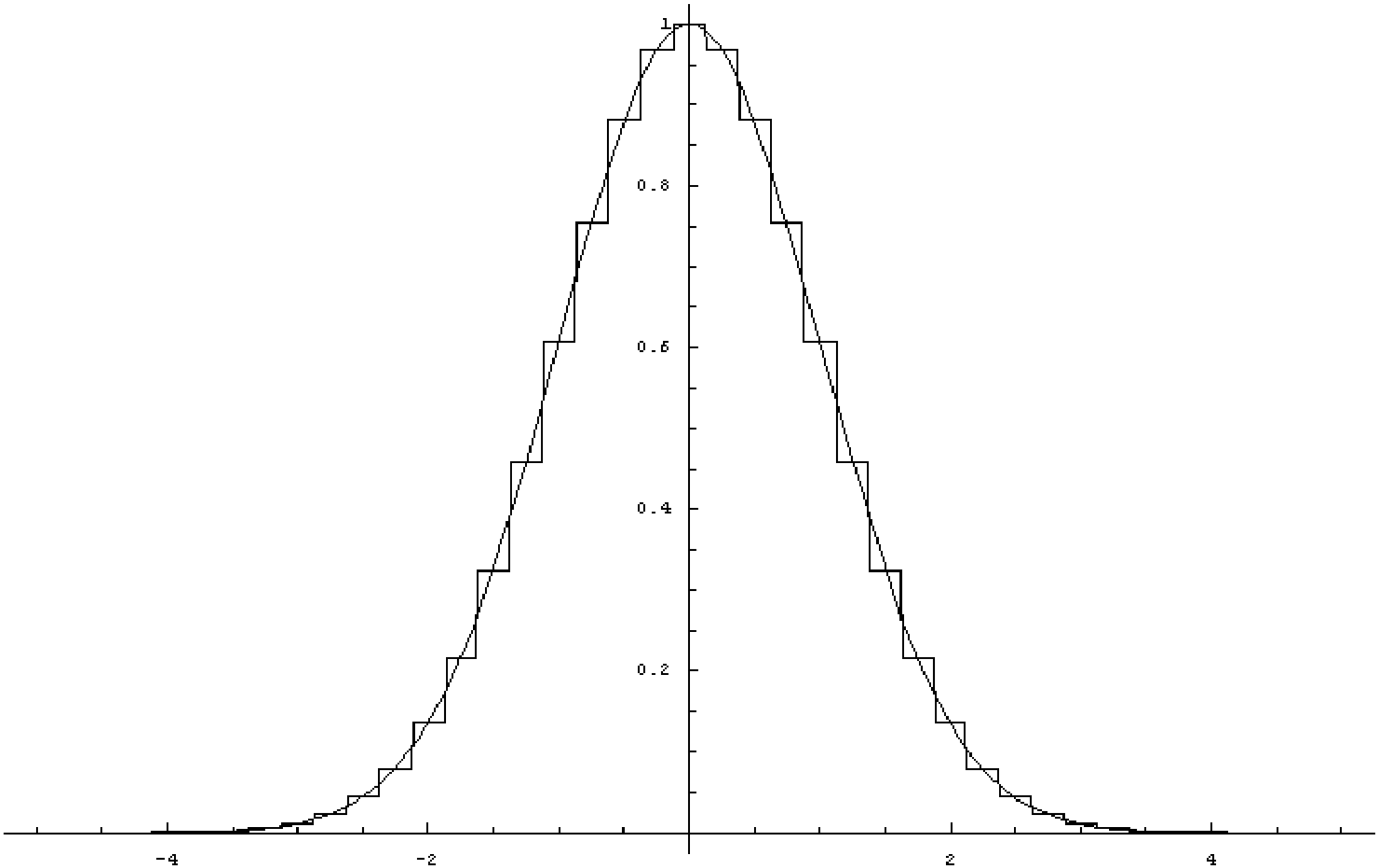
► For such functions, the error in a simple step-function approximation with interval h, is simply E(h,m) and is less than a constant (independent of h) times h^{2m+2}. Thus, the error goes to zero more rapidly than any fixed power of h.

►This leads to state-of-the-art numerical integration schemes: transform F(x) on [-1, 1] to an integral of **f(t) = F(g(t))g'(t)** on (-∞, ∞), via the *change of variable* x = g(t) for any monotonic infinitely-differentiable function such that g(x) goes +/-1 as x goes to +/-∞, while g'(x) and higher derivatives rapidly approach zero for large arguments. With x_j := g(hj) and w_j: = g'(hj), for h> 0, we have

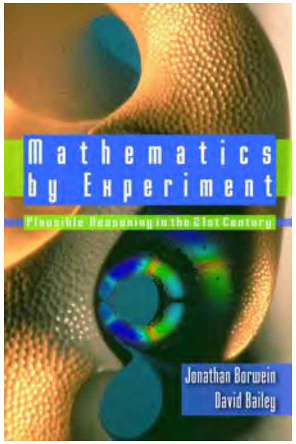
$$\begin{aligned}\int_{-1}^{1} F(x)\,dx &= \int_{-\infty}^{\infty} F(g(t))g'(t)\,dt \\ &= h\sum_{j=-\infty}^{\infty} w_j F(x_j) + E(h)\end{aligned}$$

• Even if F(x) has an infinite derivative or integrable singularity at endpoint(s) the resulting integrand will be a smooth bell-shaped function for which the prior E-Ma argument applies. Thus, the error E(h) drops very rapidly as h shrinks

Quadrature for a Bell-shaped Function



Various Choices



Various functions work well in practice

✓g(t) := tanh(t) gives rise to tanh quadrature

✓g(t) := erf(t) gives rise to ``error function'' or erf quadrature

✓g(t) := tanh(π/2 · sinh t) or g(t) := tanh (sinh t) gives rise to tanh-sinh quadrature [Takahasi, 1977]

(The cheap doubly exponential winner)

For functions to be integrated on (-∞, ∞) one can just use g(t) := sinh t, g(t) := sinh (π/2 · sinh t) or g(t) := sinh (sinh t).

``Quadratic convergence'' becomes apparent --- the number of correct digits is approximately doubled when h is halved. Table 1 shows this for the following test problems

QUADRATIC CONVERGENCE of erf

hpcs 2006

$$\mathbf{e2}:\quad \int_0^1 t^2 \arctan t\, dt = (\pi - 2 + 2\log 2)/12$$

$$\mathbf{e4}:\quad \int_0^1 \frac{\arctan(\sqrt{2+t^2})}{(1+t^2)\sqrt{2+t^2}}\, dt = 5\pi^2/96$$

$$\mathbf{e6}:\quad \int_0^1 \sqrt{1-t^2}\, dt = \pi/4$$

$$\mathbf{e8}:\quad \int_0^1 \log t^2\, dt = 2$$

$$\mathbf{e10}:\quad \int_0^{\pi/2} \sqrt{\tan t}\, dt = \pi\sqrt{2}/2$$

$$\mathbf{e12}:\quad \int_0^\infty \frac{e^{-t}}{\sqrt{t}}\, dt = \sqrt{\pi}$$

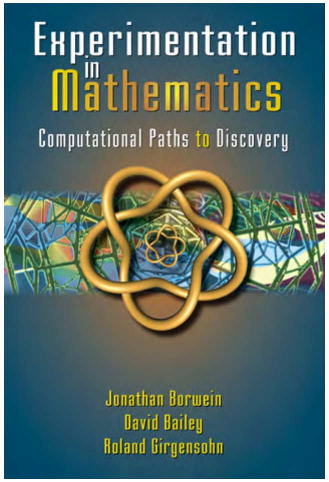
$$\mathbf{e14}:\quad \int_0^\infty e^{-t}\cos t\, dt = 1/2.$$

h	e2	e4	e6	e8
1	10^{-2}	10^{-5}	10^{-3}	10^{-3}
1/2	10^{-6}	10^{-6}	10^{-8}	10^{-10}
1/4	10^{-13}	10^{-12}	10^{-17}	10^{-21}
1/8	10^{-26}	10^{-25}	10^{-34}	10^{-43}
1/16	10^{-52}	10^{-51}	10^{-68}	10^{-87}
1/32	10^{-104}	10^{-102}	10^{-134}	10^{-173}
1/64	10^{-206}	10^{-204}	10^{-266}	10^{-348}
1/128	10^{-411}	10^{-409}	10^{-529}	10^{-696}
1/256	10^{-821}	10^{-819}	10^{-1056}	10^{-1392}

h	e10	e12	e14
1	10^{-3}	10^{-1}	10^{-1}
1/2	10^{-8}	10^{-3}	10^{-2}
1/4	10^{-16}	10^{-6}	10^{-3}
1/8	10^{-33}	10^{-11}	10^{-5}
1/16	10^{-66}	10^{-20}	10^{-10}
1/32	10^{-132}	10^{-37}	10^{-19}
1/64	10^{-264}	10^{-70}	10^{-37}
1/128	10^{-527}	10^{-132}	10^{-68}
1/256	10^{-1053}	10^{-249}	10^{-128}

Table 1. 'QUADERF' errors at successive values of h

Estimates of the Error Term



A standard estimate of the error term: If a 2π-periodic function f(z) is analytic in a strip |Im(z)| < c, the error in a trapezoidal (or step function) approx to the integral is bounded by

$$E(h) \leq \frac{4\pi M}{e^{cN} - 1},$$

where N is the number of evaluation points, $h = 2\pi / N$, and M is a bound on |f| on the complex strip

- This is interesting as it begins to explain quadratic convergence
- It is not very practical, because it requires locating complex singularities and finding a maximum on a complex strip

Doing Better

What's more, the resulting estimate is not very accurate. Consider

$$\int_{-1}^{1} \frac{dt}{1+t^2} = \frac{\pi}{2}$$

Transform by x = tanh(4sinh t) so, to a tolerance of 10^{-35}, f and a few derivatives are 0 at the endpoints of [-π,π]

The new function has a pole at 0.19763359 i.

For c = 0.197, M = 790, N = 64, h = 2 π / 64

✓ we obtain the estimate **3.32 × 10^{-2}**

By contrast, the inexpensive error estimate we introduce below with m = 1, gives **2.01832 × 10^{-5}**

Actual error in a trapezoidal approx to the integral to ten digits, is **<u>2.0183</u>003673 × 10^{-5}**

Doing Better

To derive more accurate error bounds, we need to better understand the error term in the Euler-Maclaurin formula. To that end, we state two alternate forms of the error term

Theorem 1. The error in the Euler-Maclaurin formula is

$$E(h,m) = 2(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m} \times \sum_{k=1}^{\infty} \frac{1}{k^{2m}} \int_a^b \cos[2k\pi(t-a)/h]\, D^{2m} f(t)\, dt.$$

✓ For many integrands, even the first term here is an excellent approximation to the error. In other words, we consider

$$E_1(h,m) = 2\,(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m} \times \int_a^b \cos[2\pi(t-a)/h] D^{2m} f(t)\, dt.$$

Doing Better

✓ We introduce a second approximation first discovered because of a `bug' in our program

Theorem 2. Suppose f(t) is defined on [a,b], with f(a) = f(b) = 0 and f is 2m-times cont. differentiable on [a,b], with D^k f(a) = D^k f(b) = 0 for 1 $\leq$ k $\leq$ 2m. Also h divides a and b. Let these conditions also hold with m+n replacing m. Then

$$\begin{aligned} E(h,m) &= h(-1)^{m-1}\left(\frac{h}{2\pi}\right)^{2m}\sum_{j=a/h}^{b/h} D^{2m}f(jh) \\ &+2\,(-1)^{n-1}\left(\frac{h}{2\pi}\right)^{2m+2n}\sum_{k=1}^{\infty}\left(\frac{1}{k^{2n}}+\frac{(-1)^m}{k^{2m+2n}}\right)\times \\ &\int_a^b \cos[2k\pi(t-a)/h]D^{2m+2n}f(t)\,dt. \end{aligned}$$

✓ Theorem 2 suggests using

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

Doing Better

Corollary 1 Under the hypotheses of Theorem 1 one has

$$|E(h,m) - E_1(h,m)| \leq 2\left(\zeta(2m) - 1\right)\left(\frac{h}{2\pi}\right)^{2m} \int_a^b \left|D^{2m} f(t)\right| \, dt.$$

✓This bound can be used, for instance, to establish a **rigorous ``certificate"** of the estimate $E_1(h,m)$, and thus (after computation of $E_1(h,m)$) of the quadrature itself

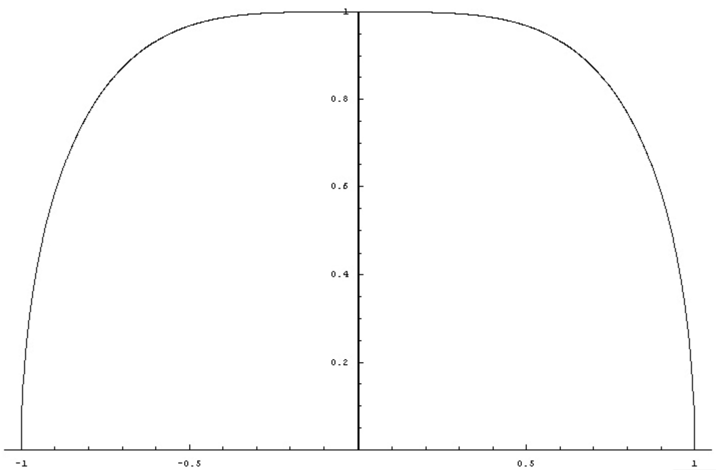
✓Other useful bounds can be derived. In particular, we mirror Corollary 1:

Corollary 2. Under the hypotheses of Theorem 2 with n=1

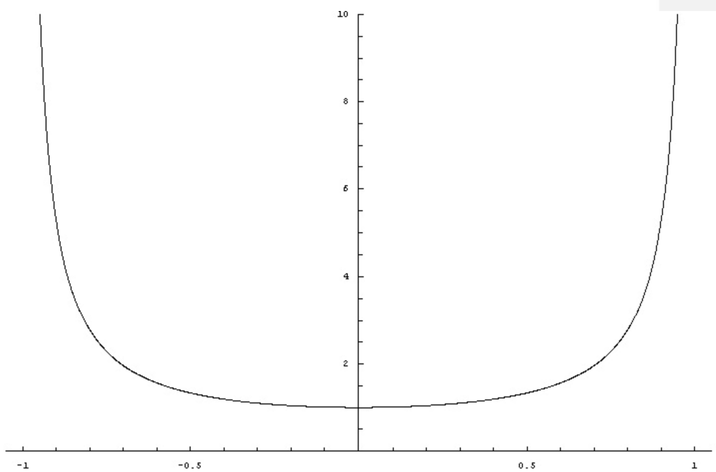
$$|E(h,m) - E_2(h,m)| \leq 2\left[\zeta(2m) + (-1)^m \zeta(2m+2)\right] \times \left(\frac{h}{2\pi}\right)^{2m} \int_a^b \left|D^{2m} f(t)\right| \, dt.$$

- This highlights what is gained by using $E_2(h,m)$ rather than $E_1(h,m)$
  - Note this is particularly advantageous when m is odd

Implementations and Tests



F_2 above and F_3 below



Tables 2 through 5 include computational analysis of $E_2(h, m)$, using test functions

$$\begin{aligned}
\mathbf{f1} &: \quad F_1(t) = 1/(1 + t^2 + t^4 + t^6) \\
\mathbf{f2} &: \quad F_2(t) = (1 - t^4)^{1/2} \\
\mathbf{f3} &: \quad F_3(t) = (1 - t^2)^{-1/2} \\
\mathbf{f4} &: \quad F_4(t) = (1 + t)^2 \sin(2\pi/(1 + t)),
\end{aligned}$$

with interval of integration. $[-1, 1]$. The tanh-sinh rule was used for quadrature. In problems f1, f2 and f4, 400-digit arithmetic was employed. In problem f3, 1100-digit arithmetic was used, although 550-digit arithmetic suffices here if one employs a "secondary epsilon" technique described in [4]. Note that $F_2(t)$ has an infinite derivative at the endpoints, and $F_3(t)$ has a blow-up singularity at the endpoints, while $F_4(t)$ represents a worst case for these methods, since it is highly oscillatory near -1. In particular, while the first two derivatives of the transformed function $f_4(t)$ tend to zero with large positive and negative arguments, the third and higher derivatives do not. (See Figure 1.)

Implementations and Tests

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$	$\lvert E(h)-E_2(h,2)\rvert$	$\lvert E(h)-E_2(h,3)\rvert$	$\lvert E(h)-E_2(h,4)\rvert$
$1/1$	-9.38039×10^{-5}	2.00740×10^{-7}	1.00302×10^{-6}	4.20595×10^{-6}	1.69621×10^{-5}
$1/2$	6.69591×10^{-8}	1.17622×10^{-15}	5.88109×10^{-15}	2.47006×10^{-14}	9.99785×10^{-14}
$1/4$	-3.92072×10^{-16}	2.48852×10^{-32}	1.24426×10^{-31}	5.22589×10^{-31}	2.11524×10^{-30}
$1/8$	-8.29506×10^{-33}	2.17847×10^{-66}	1.08924×10^{-65}	4.57479×10^{-65}	1.85170×10^{-64}
$1/16$	-7.26158×10^{-67}	4.51319×10^{-135}	2.25659×10^{-134}	9.47769×10^{-134}	3.83621×10^{-133}
$1/32$	-1.50440×10^{-135}	3.19951×10^{-272}	1.59976×10^{-271}	6.71897×10^{-271}	2.71958×10^{-270}
$1/64$	1.06650×10^{-272}	4.25792×10^{-546}	2.12896×10^{-545}	8.94163×10^{-545}	3.61923×10^{-544}

Table 4. Results for $F_3(t)=(1-t^2)^{-1/2}$ **on** $[-1,1]$**.**

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$
$1/1$	-6.45859×10^{-1}	3.54091×10^{0}
$1/2$	2.54145×10^{-2}	7.23759×10^{-1}
$1/4$	-1.69389×10^{-2}	1.00104×10^{-1}
$1/8$	-8.84080×10^{-3}	1.37392×10^{-2}
$1/16$	1.08078×10^{-3}	8.85166×10^{-4}
$1/32$	-2.39628×10^{-4}	8.44565×10^{-5}
$1/64$	-4.87134×10^{-5}	3.42934×10^{-5}

Table 5. Results for $F_4(t)=(1+t)^2\sin(2\pi/(1+t))$ **on** $[-1,1]$**.**

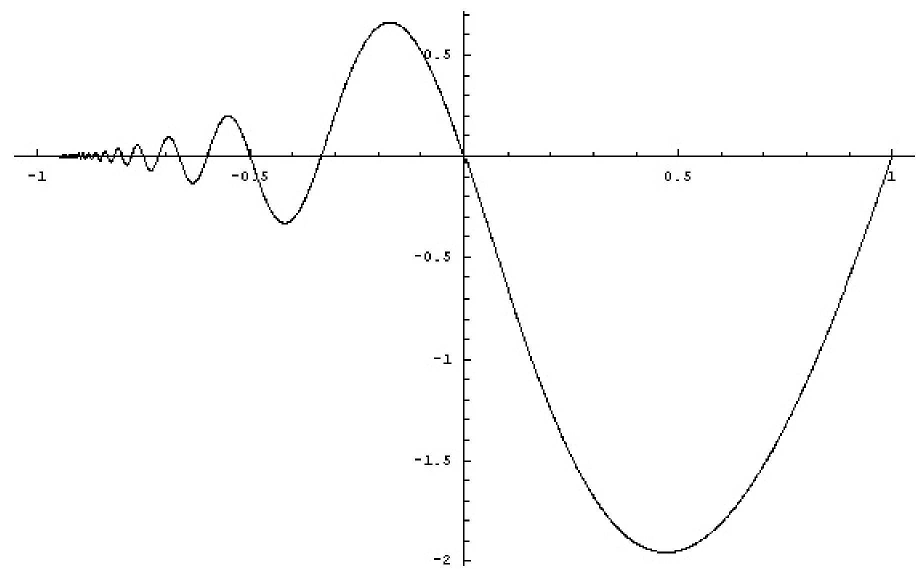


Fig 1. Test function F_4

Implementations and Tests

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$	$\lvert E(h)-E_2(h,2)\rvert$	$\lvert E(h)-E_2(h,3)\rvert$	$\lvert E(h)-E_2(h,4)\rvert$
$1/1$	5.34967×10^{-3}	9.81980×10^{-4}	4.77454×10^{-3}	1.87712×10^{-2}	6.48879×10^{-2}
$1/2$	-3.36641×10^{-4}	1.12000×10^{-7}	5.60084×10^{-7}	2.35316×10^{-6}	9.53208×10^{-6}
$1/4$	-3.73280×10^{-8}	1.67517×10^{-16}	8.37583×10^{-16}	3.51785×10^{-15}	1.42389×10^{-14}
$1/8$	5.58389×10^{-17}	2.29357×10^{-32}	1.14679×10^{-31}	4.81651×10^{-31}	1.94954×10^{-30}
$1/16$	-7.64525×10^{-33}	2.07256×10^{-64}	1.03628×10^{-63}	4.35237×10^{-63}	1.76167×10^{-62}
$1/32$	-6.90852×10^{-65}	7.23441×10^{-129}	3.61721×10^{-128}	1.51923×10^{-127}	6.14925×10^{-127}
$1/64$	$-2.41147 \times 10^{-129}$	9.08805×10^{-259}	4.54403×10^{-258}	1.90849×10^{-257}	7.72485×10^{-257}

Table 2. Results for $F_1(t) = 1/(1+t^2+t^4+t^6)$ **on** $[-1, 1]$**.**

h	$E(h)$	$\lvert E(h)-E_2(h,1)\rvert$	$\lvert E(h)-E_2(h,2)\rvert$	$\lvert E(h)-E_2(h,3)\rvert$	$\lvert E(h)-E_2(h,4)\rvert$
$1/1$	2.92136×10^{-2}	4.12347×10^{-5}	2.06449×10^{-4}	8.69796×10^{-4}	3.54584×10^{-3}
$1/2$	1.37266×10^{-5}	3.40342×10^{-11}	1.70174×10^{-10}	7.14758×10^{-10}	2.89332×10^{-9}
$1/4$	1.13445×10^{-11}	1.60476×10^{-21}	8.02380×10^{-21}	3.36999×10^{-20}	1.36405×10^{-19}
$1/8$	5.34920×10^{-22}	1.06920×10^{-41}	5.34599×10^{-41}	2.24532×10^{-40}	9.08818×10^{-40}
$1/16$	3.56399×10^{-42}	1.36460×10^{-81}	6.82298×10^{-81}	2.86565×10^{-80}	1.15991×10^{-79}
$1/32$	4.54865×10^{-82}	6.34476×10^{-161}	3.17238×10^{-160}	1.33240×10^{-159}	5.39305×10^{-159}
$1/64$	2.11492×10^{-161}	3.89818×10^{-319}	1.94909×10^{-318}	8.18618×10^{-318}	3.31345×10^{-317}

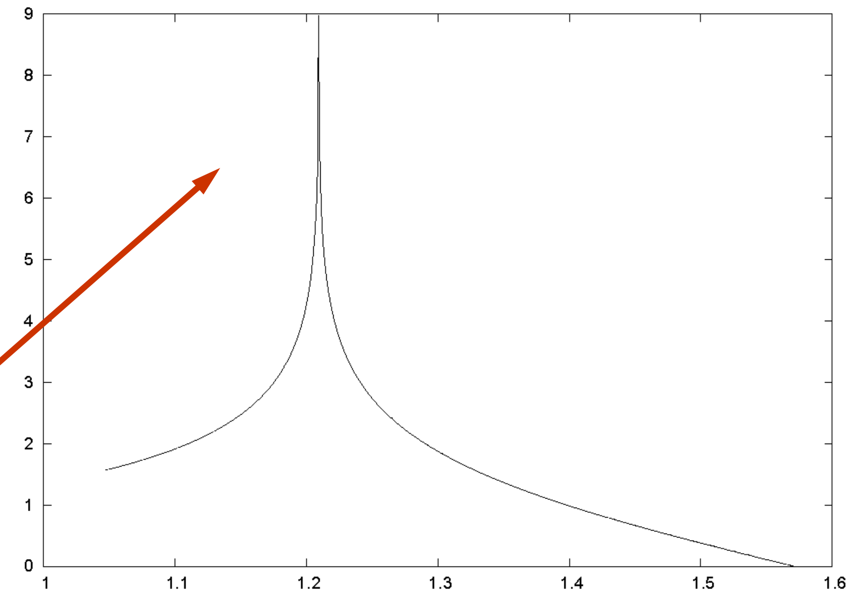
Table 3. Results for $F_2(t) = (1-t^4)^{1/2}$ **on** $[-1, 1]$**.**

A QFT Physics Example

David Broadhurst and I found the following conjectural identity in (1996):

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

This is one of 998 such identities arising out of studies in quantum field theory, in analysis of the volume of ideal tetrahedra in hyperbolic space. Such studies are currently of substantial interest to mathematical physicists, topologists and knot theorists. Note the integrand has a nasty internal singularity at t = arctan ($7^{1/2}$).



Implementation and Timing

✓run at Virginia Tech

- ✓ originally **ONLY** 800 fold speedup

✓using a stridingTanh-Sinh

✓all operations need FFT's and reduced complexity algorithms

✓ certified to 50 digits but correct to 19,995 places

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

Parallel run times (in seconds) and speedup ratios for the 20,000-digit problem

LBNL's High-Precision Software (ARPREC and QD)

- Low-level routines written in C++.
- C++ and F-90 translation modules permit use with existing programs with only minor code changes.
- Double-double (32 digits), quad-double, (64 digits) and arbitrary precision (>64 digits) available.
- Special routines for extra-high precision (>1000 dig).
- Includes common math functions: sqrt, cos, exp, etc.
- PSLQ, root finding, numerical integration.
- An interactive "Experimental Mathematician's Toolkit" employing this software is also available.

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

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

An Ising Susceptibility Integral (bis)

Bailey, Crandall and I are currently studying:

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

The first few values are known: $D_1=2$, $D_2= 2/3$, while

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

and

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

- ✓ Computer Algebra Systems can (with help) find the first 3
- ✓ D_4 is a remarkable **1977** result due to McCoy--Tracy--Wu

An Extreme Ising Quadrature

hpcs 2006

Recently Tracy asked for help 'experimentally' evaluating D_5

Using `PSLQ` this entails being able to evaluate a five dimensional integral to at least 50 or 100 places so that one can search for combinations of 6 to10 constants

✓ Monte Carlo methods can certainly not do this

✓ We are able to reduce D_5 to a horrifying several-page-long 3-D symbolic integral !

✓A 256 cpu `tanh-sinh' computation at LBNL provided 500 digits in 18.2 hours on ``Bassi", an IBM Power5 system:

A FIRST

0.0024846057623403154799505091539097496350606776424875161587076921618221378569154357537926899487245120187068721106392520511862069944997542265656264670853828412450011668223000454570326876973848961519824796130355252585151071543863811369617492242985578076280428947770278710921198111606340631254136038598401982807864018693072681098854823037887884875830583512578552364199694869146314091127363094605240934008871628387064364218612045090299733566341137276122202408834546315017113540844197840922456685046081844 68...

Conclusions

We have derived two estimates of the error in Euler-Maclaurin-based quadrature, one of which is particularly simple to implement, since it only involves summation of derivatives of the transformed function, at the same abscissas as the quadrature calculation itself.

It appears, from our results in several test problems, that the simplest instance of these estimates, namely $E_2(h,1)$, is not only adequate, but in fact very accurate once h is even modestly small.

What is more, the difference between this estimate and the actual error can be bounded with an easily computed formula, thus permitting some ``certificates'' of quadrature values computed using Euler-Maclaurin-based schemes.

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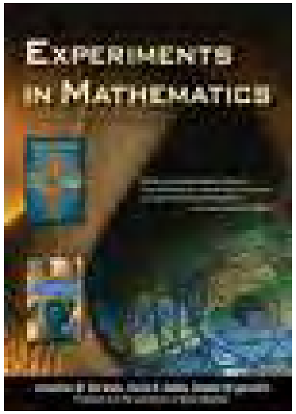

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