Future Prospects for Computer-assisted Mathematics (CMS Notes 12/05)

HIGH PERFORMANCE MATHEMATICS and its MANAGEMENT

Jonathan Borwein, FRSC www.cs.dal.ca/~jborwein
Canada Research Chair in Collaborative Technology

“intuition comes to us much earlier and with much less outside influence than formal arguments which we cannot really understand unless we have reached a relatively high level of logical experience and sophistication.”

IMA Hot Topics Workshop 12/8.9 06

The Evolution of Mathematical Communication in the Age of Digital Libraries

George Polya 1887-1987

Revised 05/12/06
ABSTRACT. Current and expected advances in computation and storage, collaborative environments and visualization make possible distant interaction in many varied and flexible ways. I'll illustrate some emerging opportunities to share research and data, seminars, classes, planning meetings and much else fully, even at a distance.

www.experimentalmath.info  www.mathresources.com

Challenges of MKM (Math Knowledge Management)
- integration of tools, inter-operability
- workable mathematical OCR
- intelligent-agents, automated use
- many IP/copyright and sociological issues
- metadata, standards and on
A. Communication, Collaboration and Computation.


B3. Inverse Symbolic Computation.

Much is still driven by particle physics, Moore’s Law and (soon) biology balanced by `commoditization’:

- **AccessGrid**
- **User controlled light paths**
- **Atlas** (LHC hunt for the Higgs Boson)
  - TRIUMF using 1000 cpu, 1Peta-byte/pa
- **Genomics and proteomics**
  - SARS decoded at Michael Smith Genome Centre

but **WalMart** already stores twice the public internet
What is HIGH PERFORMANCE MATHEMATICS?

Some of my examples will be very high-tech but most of the benefits can be had via

VOIP/SKYPE and a WEBCAM

MAPLE or MATLAB or …

A REASONABLE LAPTOP

A SPIRIT OF ADVENTURE

in almost all areas of mathematics
“If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics.” (Kurt Godel, 1951)
We shall explore various tools available for deciding what to believe in mathematics, and, using accessible often visual examples, illustrate the rich experimental tool-box mathematicians now have access to.

To explain how mathematicians may use High Performance Computation (HPC) and what we have in common with other computational scientists I shall mention various HPM problems including:

\[ \int_0^\infty \cos(2x) \prod_{n=1}^{\infty} \cos \left( \frac{x}{n} \right) \, dx = \frac{\pi}{8}, \]

which is both numerically and symbolically quite challenging .... and is answered at the end.
This picture is worth 100,000 ENIACs

The number of ENIACS needed to store the 20Mb TIF file the Smithsonian sold me

The past
"It says it's sick of doing things like inventories and payrolls, and it wants to make some breakthroughs in astrophysics."
Outline of HPMKM Talk

A. Communication, Collaboration and Computation.


B3. Inverse Symbolic Computation.

The talk ends when I do

Global digitization efforts are underway within the
International Mathematical Union
www.wdml.org

WDML
world digital mathematics library

CMS with Google
Remote Visualization via Access Grid

- The touch sensitive interactive D-DRIVE
- Immersion & Haptics
- and the 3D GeoWall

```
```
The future is here... (William Gibson)

... just not uniformly

East meets West: Collaboration goes National

Welcome to D-DRIVE whose mandate is to study and develop resources specific to distributed research in the sciences with first client groups being the following communities:

- High Performance Computing
- Mathematical and Computational Science Research
- Science Outreach
  - Research
  - Education/TV

AARMS
D-DRIVE  Jon Borwein  P. Borwein (SFU)  D. Bailey (Lawrence Berkeley)  
R. Crandall (Reed and Apple) and many others

Staff  
David Langstroth (Manager)  Scott Wilson (Systems)  
Various (SysOp)  Peter Dobscanyi (HPC)

Students  
Macklem (Parallel Optimization)  Wiersma (Analysis/NIST)  
Hamilton (Inequalities and Computer Algebra)  Ye (Quadrature)  
Paek (Federated search),  Oram (Haptics), et al

AIM (‘5S’ Secure, Stable, Satisfying) Presence at a Distance

Based on scalable  
• Topographic  
• Dynamic  
• Autonomous sustainable tools
Experimental Methodology

1. Gaining insight and intuition
2. Discovering new relationships
3. Visualizing math principles
4. Testing and especially falsifying conjectures
5. Exploring a possible result to see if it merits formal proof
6. Suggesting approaches for formal proof
7. Computing replacing lengthy hand derivations
8. Confirming analytically derived results

Comparing $-y^2 \ln(y)$ (red) to $y^2 - y^4$
The reader who wants to get an introduction to this exciting approach to doing mathematics can do no better than these books.
—Notices of the AMS

I do not think that I have had the good fortune to read two more entertaining and informative mathematics texts.
—Australian Mathematical Society Gazette

This Experiments in Mathematics CD contains the full text of both Mathematics by Experiment: Plausible Reasoning in the 21st Century and Experimentation in Mathematics: Computational Paths to Discovery in electronic, searchable form. The CD includes several “smart” enhancements, such as:

- Hyperlinks for all cross references
- Hyperlinks for all Internet URLs
- Hyperlinks to bibliographic references
- Enhanced search function, which assists one with a search for a particular mathematical formula or expression.

These enhancements significantly improve the usability of these files and the reader’s experience with the material.
Experimental Mathematics in Action

The emerging field of experimental mathematics has expanded to encompass a wide range of studies, all unified by the aggressive utilization of modern computer technology in mathematical research. This volume presents a number of case studies of experimental mathematics in action, together with some high level perspectives.

Specific case studies include:
- analytic evaluation of integrals by means of symbolic and numeric computing techniques
- evaluation of Apéry-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.


"I do not think that I have had the good fortune to read two more entertaining and informative mathematics texts."
—Gazette of the Australian Mathematical Society
The first series below was proven by Ramanujan. The next two were found & proven by Computer (Wilf-Zeilberger).

The candidates:

$$\frac{16}{\pi} = \sum_{n=0}^{\infty} r_3(n) (42n + 5) \left( \frac{1}{43} \right)^n$$

$$\frac{8}{\pi^2} = \sum_{n=0}^{\infty} r_5(n) (20n^2 + 8n + 1) \left( \frac{-1}{4} \right)^n$$

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} r_5(n) (820n^2 + 180n + 13) \left( \frac{-1}{45} \right)^n$$

Here, in terms of factorials and rising factorials:

$$\frac{32}{\pi^3} = \sum_{n=0}^{\infty} r_7(n) (168n^3 + 76n^2 + 14n + 1) \left( \frac{1}{43} \right)^n$$

The 4th is only true

$$r_N(n) := \frac{(2n)^N}{4nN} = \left( \frac{(1/2)_n}{n!} \right)^N.$$
Components include

- **AccessGrid**
- **UCLP** for
  - haptics
  - learning objects
  - visualization
- **Grid Computing**
- **Archival Storage**
  - Data Bases
  - Data Mining

Advanced Networking … (with CANARIE)
Haptics in the MLP

Haptic Devices extend the world of I/O into the tangible and tactile

To test latency issues …

We link multiple devices so two or more users may interact at a distance (BC/NS Demo April 06)

- in Museums and elsewhere
- Kinesiology, Surgery, Music, Art …

Sensible’s Phantom Omni
Coast to Coast Seminar Series (`C2C’)

Lead partners:
Dalhousie D-Drive – Halifax
Nova Scotia
IRMACS – Burnaby, British Columbia

Other Participants so far:
University of British Columbia, University of Alberta, University of Alberta, University of Saskatchewan, Lethbridge University, Acadia University, MUN, St Francis Xavier University, University of Western Michigan, MathResources Inc, University of North Carolina

Tuesdays 3:30 – 4:30 pm Atlantic Time
http://projects.cs.dal.ca/ddrive/
~ also available a forthcoming book chapter
The Experience

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
Jonathan Borwein, Dalhousie University
Mathematical Visualization

Uwe Glaesser, Simon Fraser University
Semantic Blueprints of Discrete Dynamic Systems

Peter Borwein, IRMACS
The Riemann Hypothesis

“No one explains chalk”

Jonathan Schaeffer, University of Alberta
Solving Checkers

Arvind Gupta, MITACS
The Protein Folding Problem

Przemyslaw Prusinkiewicz, University of Calgary
Computational Biology of Plants

Karl Dilcher, Dalhousie University
Fermat Numbers, Wieferich and Wilson Primes

Future Libraries will include more complex objects
The Technology

High Bandwidth Connections (CA*net) + PC Workstations + Audio/Video Equipment + Open Source Software
Institutional Requirements
(Scalable Investment)

- **Personal Nodes (1-4 people)**
  - Cost: Less than $10,000 (CA)

- **Small Group Projected Environment (2-10 people)**
  - Cost: $25,000 - $100,000 (CA)

- **Meeting Room Interactive Environment (2-20 people)**
  - Cost: $150,000 (CA)

- **Visualization Auditorium**
  - Cost: $500,000+ (CA)
"What I appreciate even more than its remarkable speed and accuracy are the words of understanding and compassion I get from it."
Outline of HPMKM Talk

A. Communication, Collaboration and Computation.


B3. Inverse Symbolic Computation.

The talk ends when I do

IMU Committee on Electronic Information and Communication

- Federated Search Tools are being developed by the International Mathematical Union (IMU)
  www.cs.dal.ca/ddrive/fwdm
- IMU Best Practices are lodged at www.ceic.math.ca
I continue with a variety of visual examples of high performance computing and communicating as part of Experimental Inductive Mathematics.

Our web site: [www.experimentalmath.info](http://www.experimentalmath.info) contains all links and references.

“Elsewhere Kronecker said \textit{``In mathematics, I recognize true scientific value only in concrete mathematical truths, or to put it more pointedly, only in mathematical formulas.''} ... I would rather say \textit{``computations''} than \textit{``formulas''}, but my view is essentially the same.”

Roots of Zeros

What you draw is what you see ("visible structures in number theory")


Striking fractal patterns formed by plotting complex zeros for all polynomials in powers of $x$ with coefficients 1 and -1 to degree 18

Coloration is by sensitivity of polynomials to slight variation around the values of the zeros. The color scale represents a normalized sensitivity to the range of values; red is insensitive to violet which is strongly sensitive.

- All zeros are pictured (at 3600 dpi)
- Figure 1b is colored by their local density
- Figure 1d shows sensitivity relative to the $x^9$ term
- The white and orange striations are not understood

A wide variety of patterns and features become visible, leading researchers to totally unexpected mathematical results

"The idea that we could make biology mathematical, I think, perhaps is not working, but what is happening, strangely enough, is that maybe mathematics will become biological!"

The TIFF on VARIOUS SCALES

Pictures are more democratic but they come from formulae
Roots in the most stable colouring
(The Sciences of the Artificial, Simons)
Ramanujan’s Arithmetic-Geometric Continued fraction (CF)

\[
R_\eta(a, b) = \frac{a}{\eta + \frac{b^2}{\eta + \frac{4a^2}{\eta + \frac{9b^2}{\eta + \ldots}}}}
\]

For \(a, b > 0\) the CF satisfies a lovely symmetrization

\[
R_\eta\left(\frac{a + b}{2}, \sqrt{ab}\right) = \frac{R_\eta(a, b) + R_\eta(b, a)}{2}
\]

Computing directly was too hard; even 4 places of \(R_1(1, 1) = \log 2\)

We wished to know for which \(a/b\) in \(\mathbb{C}\) this all held

A scatterplot revealed a precise cardioid where \(r = a/b\).

Which discovery it remained to prove?
Ramanujan’s Arithmetic-Geometric Continued fraction

Six months later we had a beautiful proof using genuinely new dynamical results. Starting from the dynamical system $t_0 := t_1 := 1$:

$$t_n = 1 - \frac{1}{n} t_{n-1} + \omega_{n-1} \left(1 - \frac{1}{n}\right) t_{n-2},$$

where $\omega_n = a^2, b^2$ for $n$ even, odd respectively—or is much more general.*

1. The Blackbox
2. Seeing convergence
3. Attractors. Normalizing by $n^{1/2}$ three cases appear
\[ \mathcal{R} = \left| \frac{\sum_{n \in \mathbb{Z}} (-1)^n q^n}{\sum_{n \in \mathbb{Z}} q^n} \right| \]

plots \(\mathcal{R}\) in disk
- black exceeds 1
- lighter is lower

I only roughly understand the self-similarity

\(\checkmark\) related to Ramanujan’s continued fraction
\(\checkmark\) took several hours to print
\(\checkmark\) Crandall/Apple has parallel print mode
Why should I refuse a good dinner simply because I don't understand the digestive processes involved?

Oliver Heaviside (1850 - 1925)

when criticized for his daring use of operators before they could be justified formally
"What it comes down to is our software is too hard and our hardware is too soft."
Outline of HPMKM Talk

A. Communication, Collaboration and Computation.


B3. Inverse Symbolic Computation.

The talk ends when I do

IMU Committee on Electronic Information and Communication

- Federated Search Tools are being developed by the International Mathematical Union (IMU)
  www.cs.dal.ca/ddrive/fwdm

- IMU Best Practices are lodged at
  www.ceic.math.ca

- A Registry of Digital Journals is now available
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 $\alpha$ is algebraic of degree $d$ and length $l$ (coefficient sum in absolute value).

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

**Example** (MAA, April 2005). Prove that

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

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

A fully symbolic Maple proof followed. QED $|\beta - 1| < 1/(32\lambda) \leftrightarrow \beta = 1$
Central to my work - with Dave Bailey - meshed with visualization, randomized checks, many web interfaces and

- Massive (serial) Symbolic Computation
  - Automatic differentiation code
- Integer Relation Methods
- Inverse Symbolic Computation

Other useful tools:
- Parallel Maple
- Sloane’s online sequence database
- Salvy and Zimmerman’s generating function package ‘\textit{gfun}’
- Automatic identity proving: Wilf-Zeilberger method for hypergeometric functions
Greetings from the On-Line Encyclopedia of Integer Sequences!

Integrated real-time use
- moderated
- 120,000 entries
- grows daily
- AP book had 5,000

An Exemplary Database

ID Number: A000055 (Formerly M0791 and M0299)
Sequence: 1, 1, 1, 2, 3, 6, 11, 23, 47, 106, 235, 551, 1,301, 3,159, 7,741, 19, 320, 48, 629, 12,386, 31, 795, 82, 3065, 214, 4505, 562, 375, 14, 6820, 74, 392, 99897, 104, 69890, 279, 993450, 751, 065450, 202, 3443032, 5469566585, 14830871802, 403, 3829030, 109972410221

Name: Number of trees with n unlabeled nodes.
Comments: Also, number of unlabeled 2-gonal 2-trees with n 2-gons.
N. L. Biggs et al., Graph Theory 1736–1936, Oxford, 1976, p. 49.

Links:
- P. J. Cameron, Sequences realized by oligomorphic permutation groups J. Integ. Seqs. Vol. 3 (2000) #00.1.6
- Steven Finch, Otter's Tree Enumeration Constants
- E. N. Rains and N. J. A. Sloane, On Cayley's Enumeration of Alkanes (or 4-Valent Trees)
- N. J. A. Sloane, Illustration of initial terms
- E. Weisstein, Link to a section of The World of Mathematics.

Index entries for sequences related to trees
Index entries for "core" sequences


Formula: G.f.: A(x) = 1 + T(x) - T^2(x) / 2 + T(x^2) / 2, where T(x) = x + x^2 + 2x^3 + ...
\[ A_1(z) = A_1(0) \left( 1 + \frac{1}{3} z^3 + \frac{1.4}{6} z^6 + \frac{1.4.2}{9} z^9 + \cdots \right) + A_1'(0) \left( z + \frac{2}{4} z^4 + \frac{2.5 z^7}{7!} + \frac{2.5.8 z^{10}}{10!} + \cdots \right) \]

\[ A_1'(z) = A_1'(0) \left( 1 + \frac{2}{31} z^3 + \frac{2.5 z^6}{6!} + \frac{2.5.8 z^9}{9!} + \cdots \right) + A_1(0) \left( \frac{1}{21} z^2 + \frac{1.4 z^5}{5!} + \frac{1.4.7 z^8}{8!} + \cdots \right) \]

\[ B_1(z) = B_1(0) \left( 1 + \frac{1}{3} z^3 + \frac{1.4}{6} z^6 + \frac{1.4.7}{9} z^9 + \cdots \right) + B_1'(0) \left( z + \frac{2}{4} z^4 + \frac{2.5 z^7}{7!} + \frac{2.5.8 z^{10}}{10!} + \cdots \right) \]

\[ B_1'(z) = B_1'(0) \left( 1 + \frac{2}{31} z^3 + \frac{2.5 z^6}{6!} + \frac{2.5.8 z^9}{9!} + \cdots \right) + B_1(0) \left( \frac{1}{21} z^2 + \frac{1.4 z^5}{5!} + \frac{1.4.7 z^8}{8!} + \cdots \right) \]
Multiplication

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

... in ranges from 100 to 1,000,000,000,000 digits
- The other operations via Newton’s method \( \times, \div, \sqrt{\cdot} \)
- Elementary and special functions via Elliptic integrals and Gauss AGM

For example:

\[
\begin{align*}
(a + c \cdot 10^N) \times (b + d \cdot 10^N) &= ab + (ad + bc) \cdot 10^N + cd \cdot 10^{2N} \\
&= ab + \{(a + c)(b + d) - ab - cd\} \cdot 10^N + cd \cdot 10^{2N}
going three multiplications
\]

FFT multiplication of multi-billion digit numbers reduces centuries to minutes. Trillions must be done with Karatsuba!
Newton’s Method for Elementary Operations and Functions

1. Doubles precision at each step
   Newton is self correcting and quadratically convergent

2. Consequences for work needed:
   \[
   x \leftarrow x(2 - xA) \\
   x \leftarrow 1/2 x (3 - x^2 A)
   \]
   \[
   '\div = 4 \times' : 1/x = A \\
   '\sqrt{\cdot} = 6 \times' : 1/x^2 = A
   \]

3. For the logarithm we approximate by elliptic integrals (AGM) which admit quadratic transformations: near zero
   \[
   \frac{d}{dk} K(k) \sim \log \left(\frac{4}{k}\right)
   \]

4. We use Newton to obtain the complex exponential
   So all elementary functions are fast computable
The following integrals arise in Ising theory of mathematical physics:

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

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):

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

\[
C_4 = 14\zeta(3)
\]

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

and more - via PSLQ and the Inverse Calculator to which we now turn.
A. Communication, Collaboration and Computation.


B3. Inverse Symbolic Computation.

The talk ends when I do.
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.  
  *Science* Oct 2006
- PSLQ was named one of ten “algorithms of the century” by *Computing in Science and Engineering*.
- High precision arithmetic software is required: at least \(d \times n\) 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

\[ B_3 = 3.54409035955 \ldots \text{ is third bifurcation point of the logistic iteration of chaos theory:} \]
\[ x_{n+1} = rx_n(1 - x_n) \]
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

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

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

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

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

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

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

2. reduced as hoped

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

3. was easily computer proven (Wilf-Zeilberger)

MAA: human proof?
Wilf-Zeilberger Algorithm is a form of automated telescoping:
\[
\sum_{n=1}^{\infty} \frac{1}{n(n+1)} = \sum_{n=1}^{\infty} \left\{ \frac{1}{n} - \frac{1}{n+1} \right\} = 1
\]

✓ AMS Steele Research Prize winner. In Maple 9.5 set:

\[
F := \frac{(3n + k - 1)! (n + k)! (-n + k - 1)! (2n)! (n - 1/2)! (1/4)^k}{(3n - 1)! n! (-n - 1)! (2n + k)! (n - 1/2 + k)! k!}, \quad r := \frac{\binom{2n}{n}}{\binom{3n}{n}}
\]

and execute:

```maple
> with(SumTools[Hypergeometric]):
> WZMethod(F,r,n,k,'certify'): certify;
```

which returns the certificate

\[
\begin{array}{c}
/ \quad 2 \\
\{11 n + 1 + 6 n + k + 5 k n/ k \\
- \quad \text{-------------------------}
\}
\end{array}
\]

\[
3 (n - k + 1) (2 n + k + 1) n
\]

This proves that summing \(F(n,k)\) over \(k\) produces \(r(n)\), as asserted.
My brother made the observation that this log formula allows one to compute binary digits of \( \log 2 \) without knowing the previous ones! (a BBP formula)

This reduced to which Maple, Mathematica and humans can easily prove. A triumph for “reverse engineered mathematics” [algorithm design]

Bailey, Plouffe and he hunted for such a formula for Pi. Three months later the computer - doing bootstrapped PSLQ hunts - returned:

\[
\log 2 = \sum_{n=1}^{\infty} \frac{1}{k \cdot 2^k}
\]

No such formula exists base-ten (provably)

Finalist for the $100K Edge of Computation Prize won by David Deutsch (2005)
The pre-designed Algorithm ran the next day

Now built into some compilers!
Bailey and Crandall observed that BBP numbers most probably are normal and make it precise with a hypothesis on the behaviour of a dynamical system. For example, Pi is normal in hexadecimal if the iteration below, starting at zero, is uniformly distributed in $[0,1]$

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

Consider the hex digit stream:

$$d_n = \lfloor 16x_n \rfloor$$

We have checked this gives first million hex-digits of Pi. Is this always the case? The weak Law of Large Numbers implies this is very probably true!
IF THERE WERE COMPUTERS IN GALILEO'S TIME
Outline of HPMKM Talk

A. Communication, Collaboration and Computation.


B3. Inverse Symbolic Computation.

The talk ends when I do.

Inverse Symbolic Computation

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**

Expressions that are not numeric like \(\ln(P\sqrt{2})\) are evaluated in **Maple** in symbolic form first, followed by a floating point evaluation followed by a lookup.
Donald Knuth* asked for a closed form evaluation of:

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

The answer is Gonnet’s Lambert’s W which solves

$$W \exp(W) = x$$

We can know the answer first.

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

The answer is

Gonnet’s

Lambert’s W

which solves

$$W \exp(W) = x$$

The answer

is

Gonnet’s

Lambert’s W

which solves

$$W \exp(W) = x$$

The answer is

Gonnet’s

Lambert’s W

which solves

$$W \exp(W) = x$$

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 Lookup' gives:

\[ K = 0.08406950872765600 \]

\[ \text{Value to be looked up: } 0.08406950872765600e-1 \]

Answers are given from shortest to longest description.
Quadrature I. Hyperbolic Knots

\[
\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \overset{?}{=} L_{-7}(2) \quad (@)
\]

where

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

"Identity" (@) has been verified to 20,000 places. I have no idea of how to prove it.

The easiest of 998 empirical results (PSLQ, PARI, SnapPea) linking physics/topology (LHS) to number theory (RHS).
[JMB-Broadhurst, 1996]
Expected and unexpected scientific spinoffs

- **1986-1996.** Cray used quartic-Pi to check machines in factory
- **1986.** Complex FFT sped up by factor of two
- **2002.** Kanada used hex-pi (20hrs not 300hrs to check computation)
- **2005.** Virginia Tech (this integral pushed the limits)
- **2006.** A 3D Ising integral took 18.2 hrs on 256 cpus (for 500 places)
- **1995- Math Resources** (another lecture)

The integral was split at the nasty interior singularity
The sum was `easy'.
All fast arithmetic & function evaluation ideas used

---

**Run-times and speedup ratios on the Virginia Tech G5 Cluster**

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

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

---

**Extreme Quadrature … 20,000 Digits (50 Certified) on 1024 CPUs**
Quadrature II. Ising Susceptibility Integrals

Bailey, Crandall and I recently studied:

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

The first few values are known: \( D_1 = 2, \ D_2 = 2/3, \)
while
\[ D_3 = 8 + \frac{4}{3} \pi^2 - 27 \ \zeta(3) \]

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

\( D_4 \) is a remarkable 1977 result due to McCoy--Tracy--Wu.

Computer Algebra Systems can (with help) find the first 3
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 250 places so that one can search for combinations of 6 to 15 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

18.2 hours on ```Bassi``, an IBM Power5 system:

```plaintext
0.00248460576234031547995050915390974963506067764248751615870769
216182213785691543575379268994872451201870687211063925205118620
699449975422656562646708538284124500116682230004545703268769738
489615198247961303552525851510715438638113696174922429855780762
804289477702787109211981116063406312541360385984019828078640186
930726810988548230378878848758305835125785523641996948691463140
911273630946052409340088716283870643642186120450902997335663411
372761220240883454631501711354084419784092245668504608184468...
```
A numerically challenging integral tamed

\[ \int_0^\infty \cos(2x) \prod_{n=1}^\infty \cos\left(\frac{x}{n}\right) \, dx = \frac{\pi}{8}. \]

Now \( \pi/8 \) equals

\[ 0.392699081698724154807830422909937860524645434 \]

while the integral is

\[ 0.3926990816987241548078304229099378605246461749 \]

A careful tanh-sinh quadrature proves this difference after 43 correct digits

Fourier analysis explains this happens when a hyperplane meets a hypercube (LP)
REFERENCES


“The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it.”
