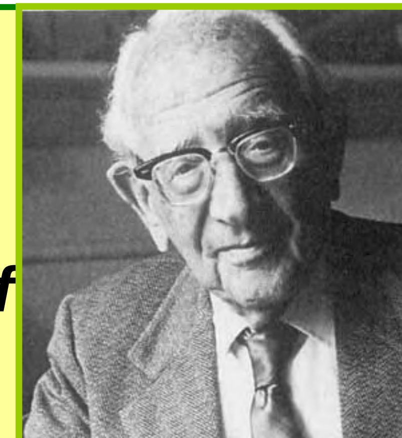
Future Prospects for Computer-assisted Mathematics (CMS Notes 12/05)

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



George Polya 1887-1985

The Evolution of Mathematical Communication in the Age of Digital Libraries

DALHOUSIE UNIVERSITY
Inspiring Minds
Faculty of Computer Science

Revised 08/12/06

ACES. Advanced Collaborative Environments

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, defenses, planning and hiring meetings and much else <u>fully</u>, even at a distance.**

URLS. http://projects.cs.dal.ca/ddrive http://users.cs.dal.ca/~jborwein

www.experimentalmath.info www.mathresources.com (corporate)

Challenges of MKM (Math Knowledge Management)

- integration of tools, inter-operability
- workable *mathematical OCR*
- intelligent-agents, automated use
- <u>many</u> IP/copyright (*caching*) and social issues
- metadata, standards and on

www.mkm-ig.org

Outline of HPMKM Talk

A. Communication, Collaboration and Computation.

B1. Visual Data Mining in Mathematics (old and new).

B2. Integer Relation Methods (and their numerics).

B3. Inverse Symbolic Computation.

Most Mathematics is done by non-professionals

The talk ends when I do

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

Tom Paxton: `Error type 411`

`I typed 411`

- Almost three-fourths of adults who do use instant messages still communicate with e-mail more often. Almost three-fourths of teens send instant messages more than e-mail.
- More than half of the teens who use instant messages send more than 25 a day, and one in five send more than 100. Three-fourths of adult users send fewer than 25 instant messages a day.
- Teen users (30 per cent) are almost twice as likely as adults (17 per cent) to say they can't imagine life without instant messaging.
- When keeping up with a friend who is far away, teens are most likely to use instant messaging, while adults turn first to e-mail.
- **About a fifth of teen IM users have used IM to ask for or accept a date. Almost that many, 16 per cent, have used it to break up with someone.**
- A bow to the traditional: When sharing serious or confidential news, both teens and adults prefer to use the telephone, the poll said.

The survey of 1,013 adults and 500 teens was conducted online by Knowledge Networks from Nov. 30 to Dec. 4. The margin of sampling error for the adults was

2006 | 8:36 AM ET The Associated Press

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

A FEW PLUGINS

MAPLE or MATLAB or …

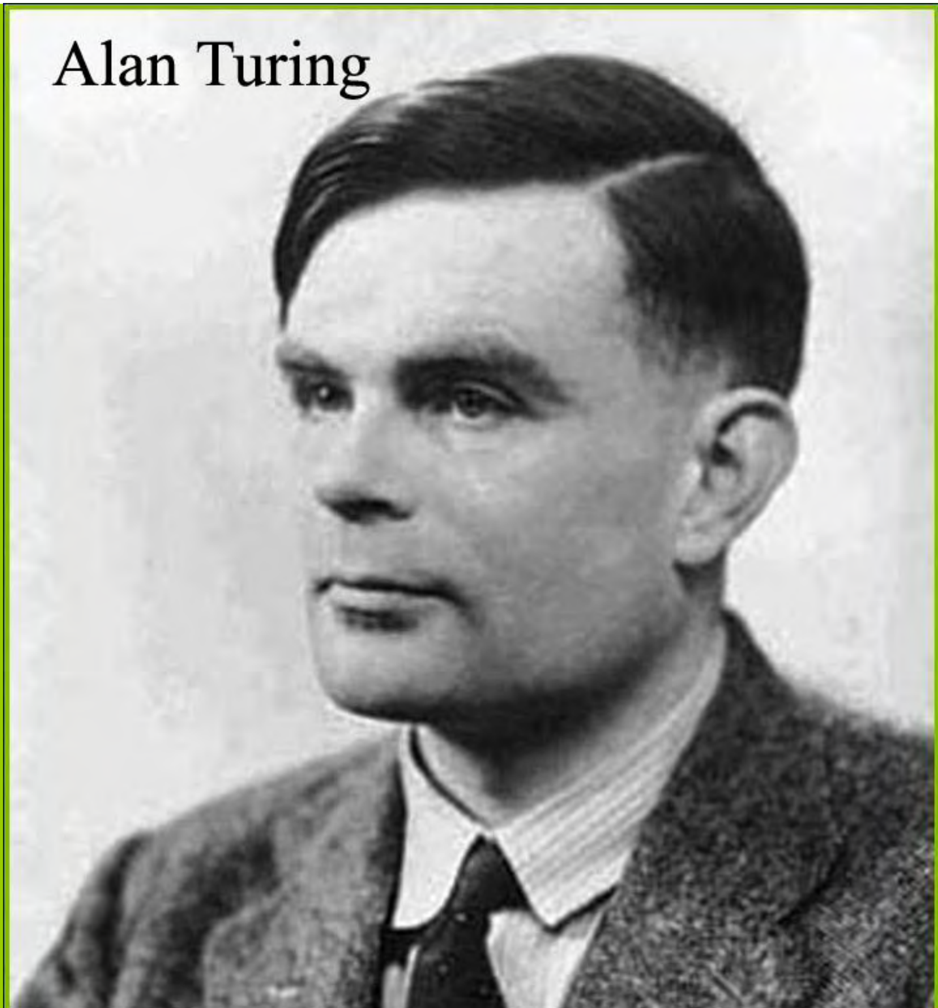
A REASONABLE LAPTOP

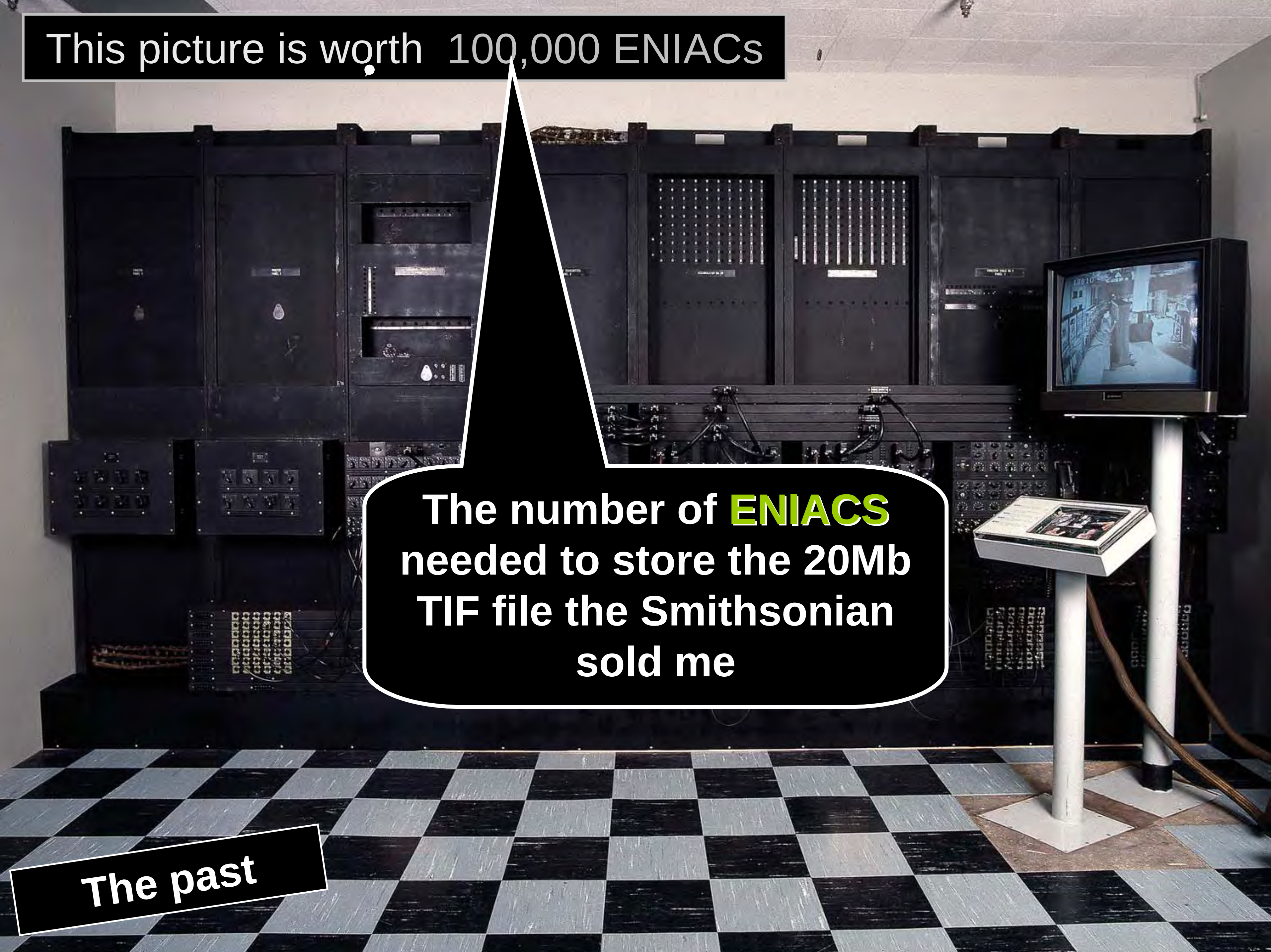
A SPIRIT OF ADVENTURE

in almost all areas of mathematics.
I talk as an avid IT consumer

Induction

"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)




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 break-throughs in astrophysics."

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B3. Inverse Symbolic Computation.

Cognitive skills are changing: (Stroop) design for our kids not ourselves

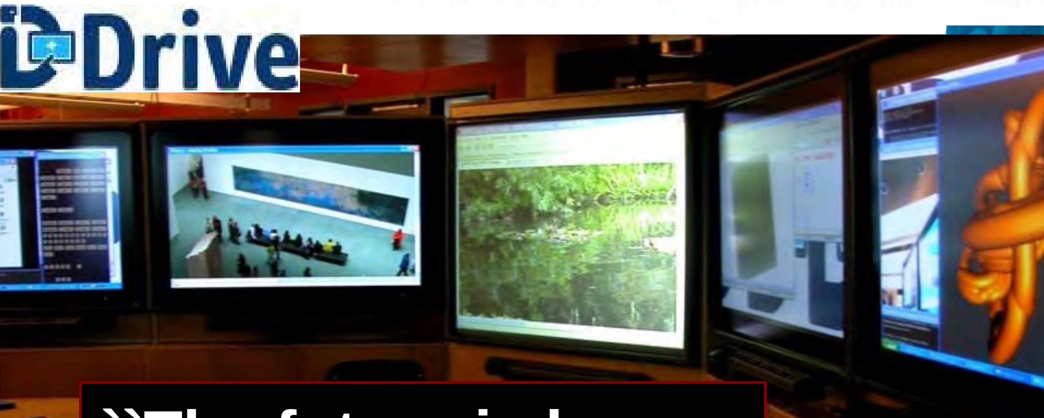
The talk ends when I do

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

WDML
world digital mathematics library

CMS with **Google**

Drive



``The future is here… (William Gibson) … just not uniformly''

Remote Visualization via **Access Grid**

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

Dalhousie Distributed Research Institute and Virtual Environment

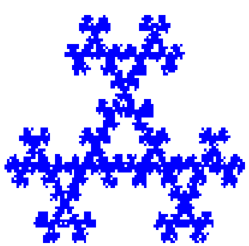
East meets West: Collaboration goes National

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

Atlantic Computational Excellence Network

ACEnet

- 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 Opt/FWDM) Wiersma (Analysis/ NIST) Hamilton (Inequalities and Computer Algebra) Ye (Parallel 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 Mathodology

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

MATH LAB

Computer experiments are transforming mathematics

BY ERICA KLARREICH

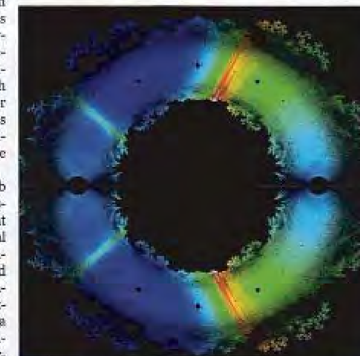
Science News 2004

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.

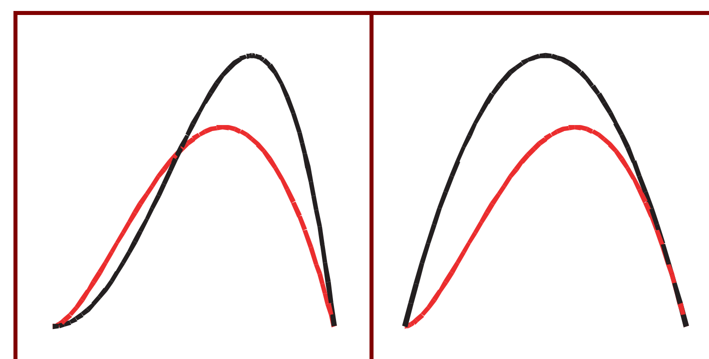
For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

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.

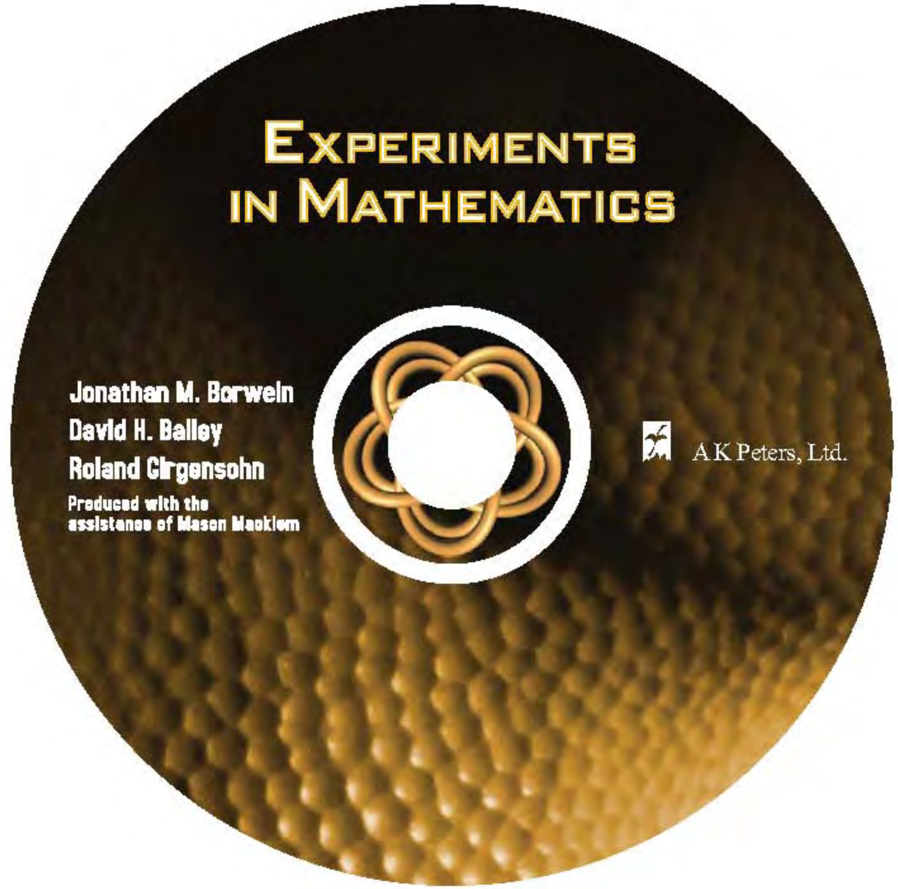
Like today's mathematicians, math experimenters in the late 19th century used computers—but in those days, the word referred to people with a special facility for calcu-

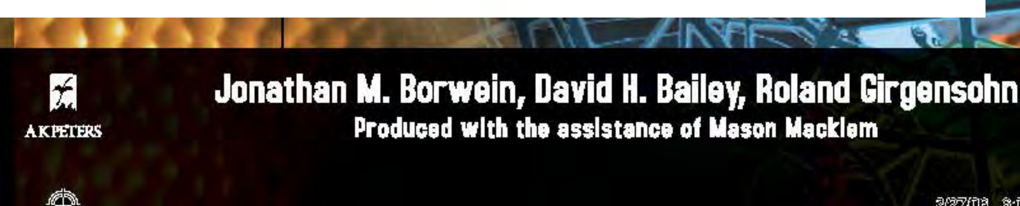


Comparing $-y^2\ln(y)$ (red) to $y-y^2$ and y^2-y^4

2006: SELF-ADVERTISEMENT

Some math search tools added





March 2007

Experimental Mathematics in Action

David H. Bailey, Jonathan M. Borwein, Neil Calkin,
Roland Girgensohn, Russell Luke, Victor Moll

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 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.

September 2006; ISBN 1-56881-271-X; Hardcover; Approx. 200 pp.; $39.00

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

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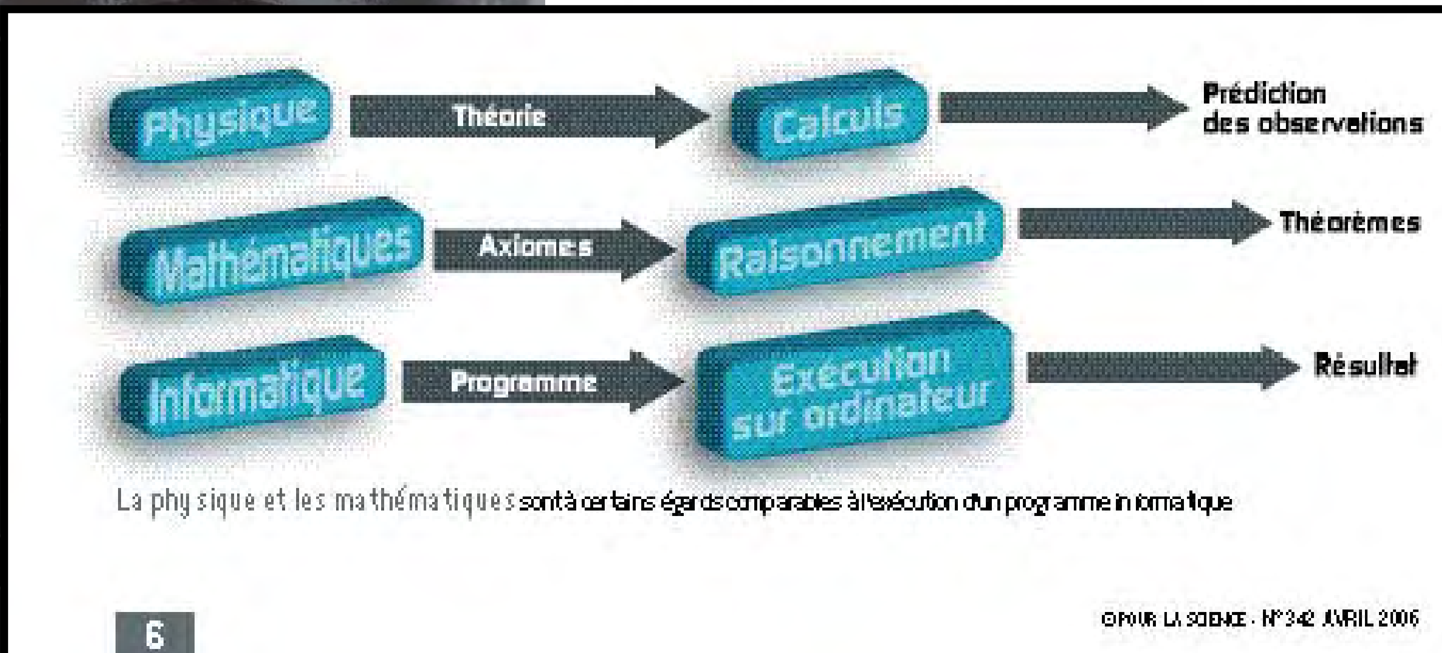

La physique et les mathématiques sont à certains égards comparables à l'exécution d'un programme informatique

ts to get an introduction
n [this book]."
— *Notices* of the AMS

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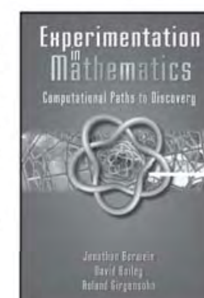


True, but why ?

The first series below was proven by Ramanujan. The next two were found & proven by Computer (Wilf-Zeilberger).

The candidates:

$$\frac{16}{\pi} = \sum_{n=0}^{\infty} r_3(n)\,(42n+5)\left(\frac{1}{4^3}\right)^n$$

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

$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} r_5(n)\,(820n^2+180n+13)\left(\frac{-1}{4^5}\right)^n$$

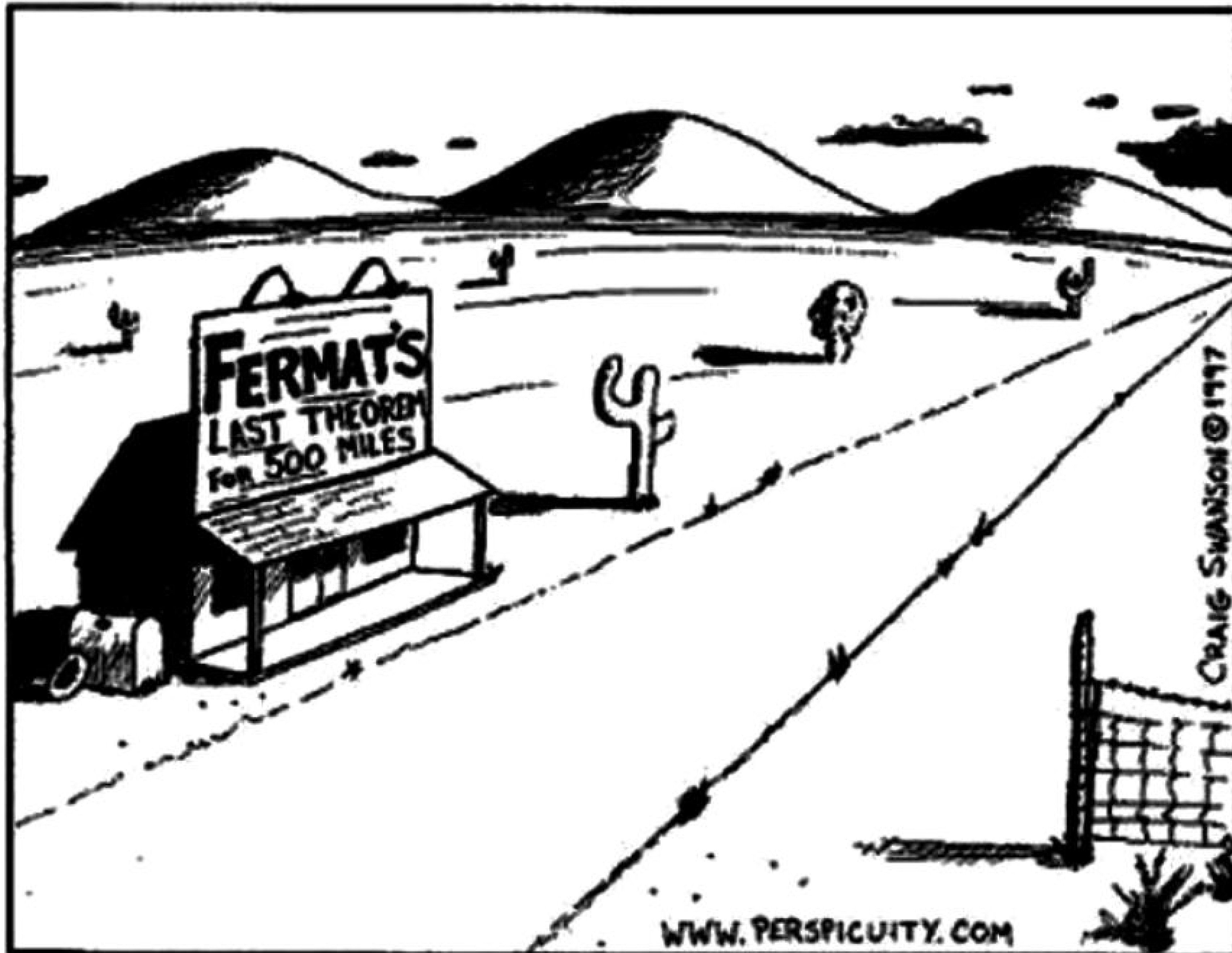
$$\frac{32}{\pi^3} = \sum_{n=0}^{\infty} r_7(n)\,(168n^3+76n^2+14n+1)\left(\frac{1}{4^3}\right)^n$$

Here, in terms of factorials and rising factorials:

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

The 4th is only true

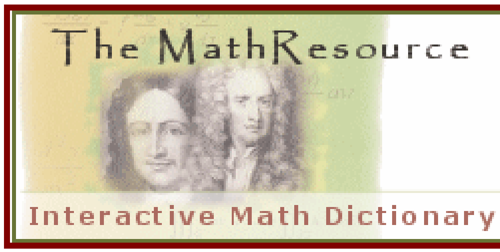
$$r_N(n) \sim_n \frac{1}{n^{N/2}}$$

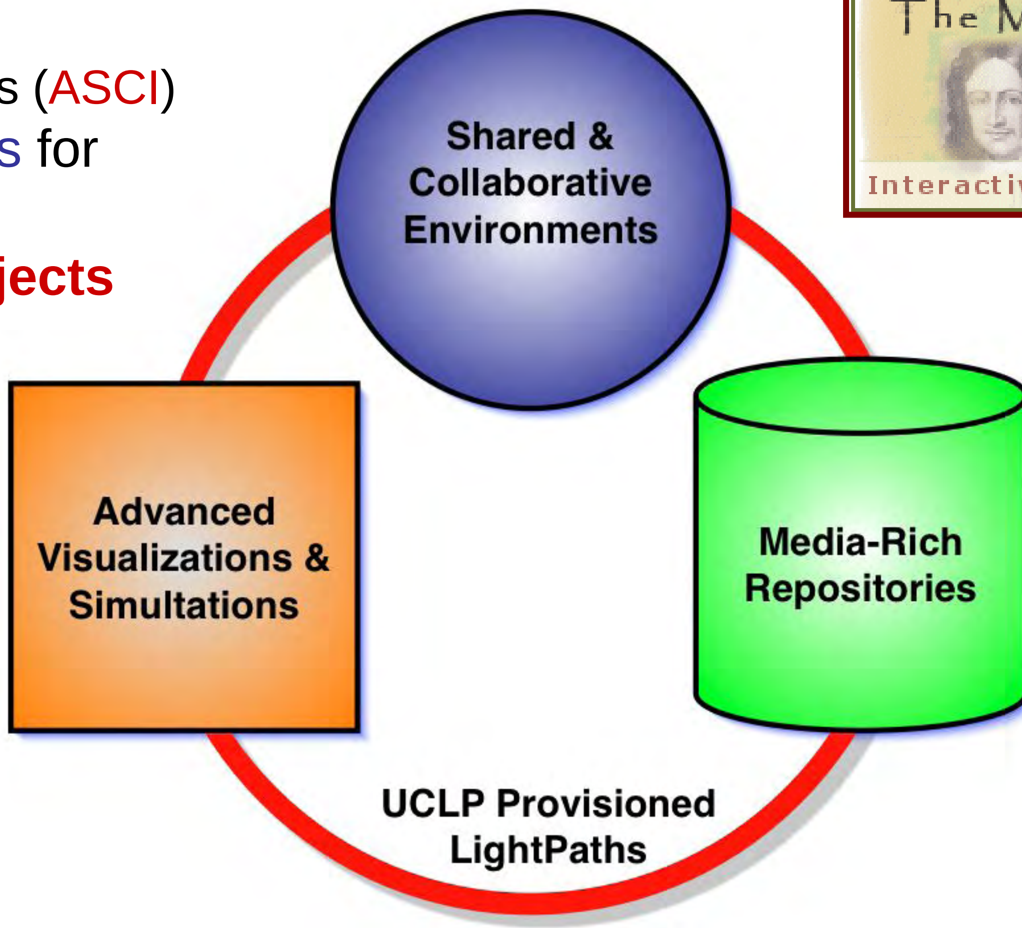

FERMAT'S
LAST THEOREM
FOR 500 MILES
CRAIG SWANSON © 1997
WWW.PERSPICUITY.COM

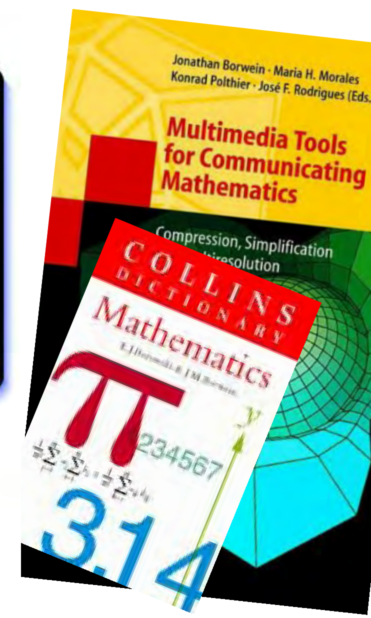
Advanced Networking … (with CANARIE)

Components include

- **AccessGrid**
  - ✓ shared courses (ASCI)
- **UCLP** vs packets for
  - ✓ haptics
  - ✓ **learning objects**
  - ✓ visualization
- **Grid Computing**
- **Archival Storage**
  - ✓ **Data Bases**
  - ✓ **Data Mining**

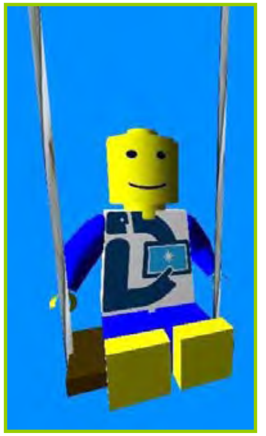






Haptics in the MLP

D-DRIVE Doug our haptic mascot



Drive
Dalhousie Distributed Research Institute and Virtual Environment

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, Aware Homes, elsewhere
- Kinesiology, Surgery, Music, Art …

Sensable's **Phantom Omni**

Coast to Coast Seminar Series ('C2C')

AG Prototype for Atlantic Shared Curriculum Initiative (ASCI)

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 a forthcoming book chapter

The Experience

Fully Interactive multi-way audio and visual

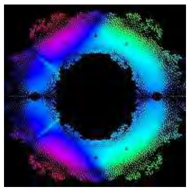
Given good bandwidth audio is much harder

The closest thing to being in the same room

Steve Watt could be here

Shared Desktop for viewing presentations or sharing software

Dalhousie Distributed Research Institute and Virtual Environment



Jonathan Borwein, Dalhousie University
Mathematical Visualization

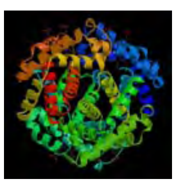
High Quality Presentations

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



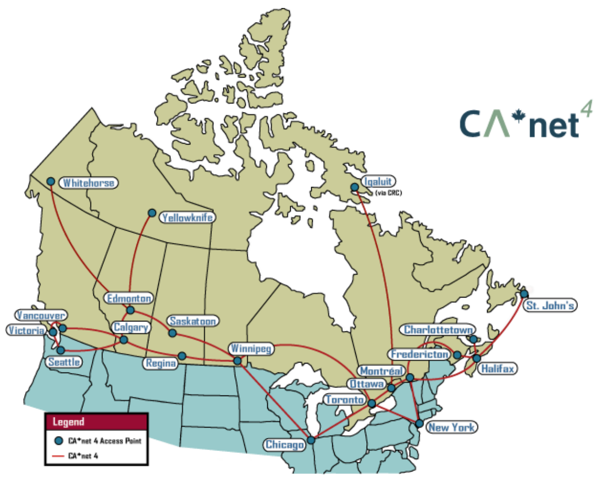
Arvind Gupta, MITACS
The Protein Folding Problem

Przemyslaw Prusinkiewicz, University of Calgary
Computational Biology of Plants

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

Future Libraries must include more complex objects

Dalhousie Distributed Research Institute and Virtual Environment



The **scalable** Technology

High Bandwidth Connections (CA*net)

+

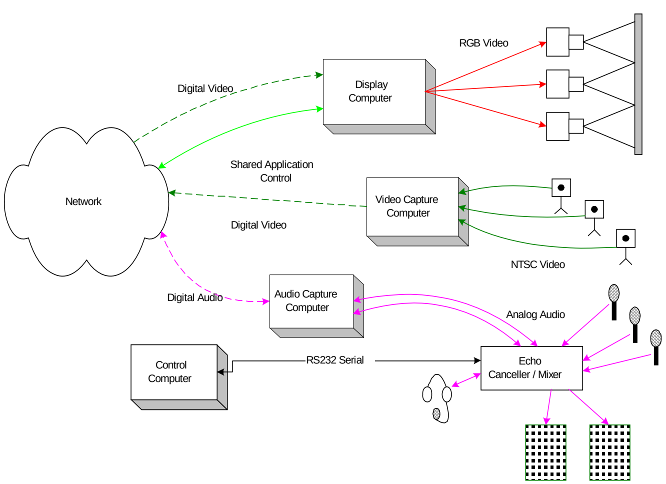
PC Workstations

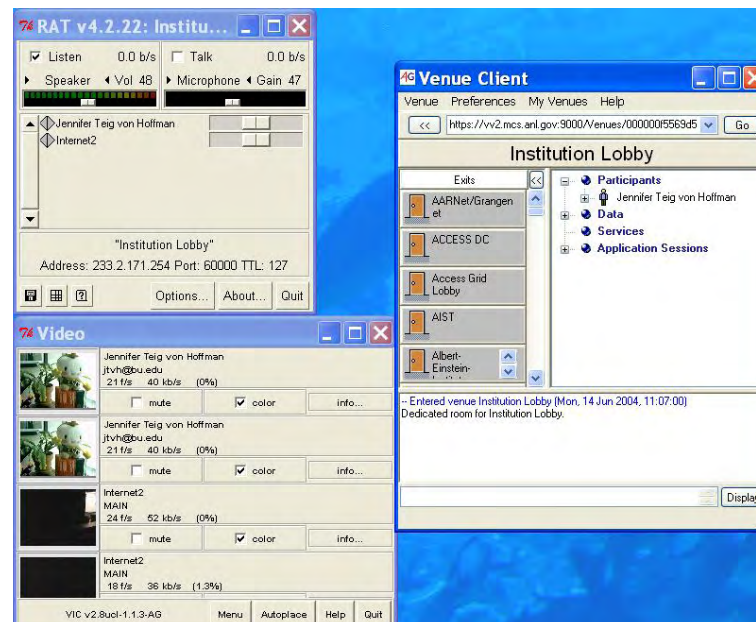
+

Audio/Video Equipment

+

Open Source Software

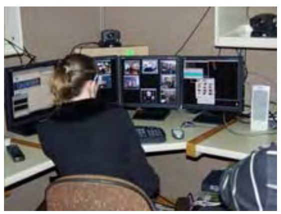


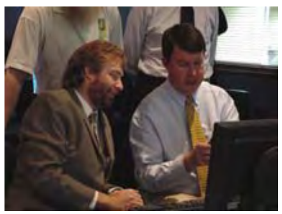


Dalhousie Distributed Research Institute and Virtual Environment

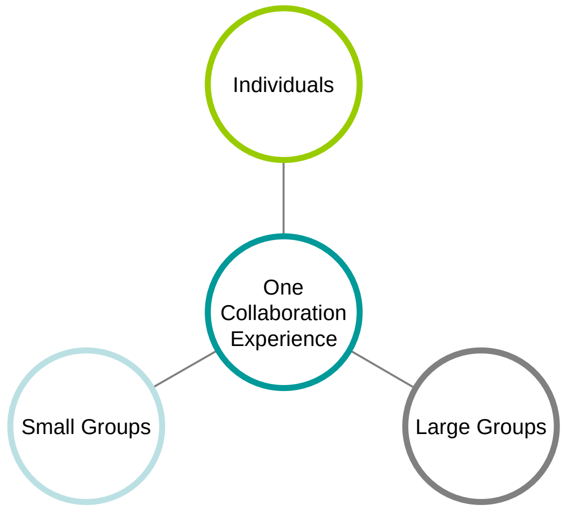
Institutional Requirements
(Scalable Investment)

Personal Nodes
(1-4 people)





Cost: Less than $10,000 (CA)



Meeting Room
Interactive Environment
(2-20 people)

Cost: $150,000 (CA)

Small Group
Projected Environment
(2-10 people)

Cost: $25,000 - $100,000 (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."

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IMU Committee on Electronic Information and Communication

- **Federated Search Tools** have been developed by the **International Mathematical Union (IMU)** **www.cs.dal.ca/ddrive/fwdm**
- **IMU Best Practices** are lodged at **www.ceic.math.ca**
- **Digital Journal Registry** **www.wdml.org** released Oct 2006

The David Borwein CMS Career Award

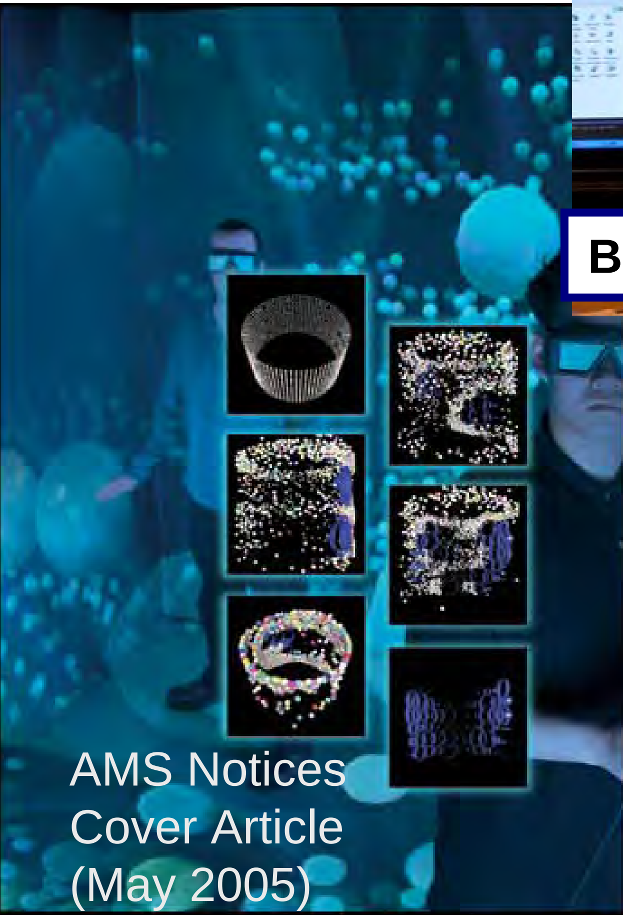
$$= \sum_{n,m,p}{}' \frac{(-1)^{n+m+p}}{\sqrt{n^2+m^2+p^2}}$$

This polished solid silicon bronze sculpture is inspired by the work of David Borwein, his sons and colleagues, on the conditional series above for salt, Madelung's constant. This series can be summed to give uncountably many constants; one is Madelung's constant for sodium chloride.

This constant is a period of an elliptic curve, a real surface in four dimensions. There are uncountably many ways to imagine that surface in three dimensions; one has negative gaussian curvature and is the tangible form of this sculpture. (As described by the artist.)

5 Smart Shared-Screens

Being emulated by the Canadian Kandahar mission



AMS Notices Cover Article (May 2005)

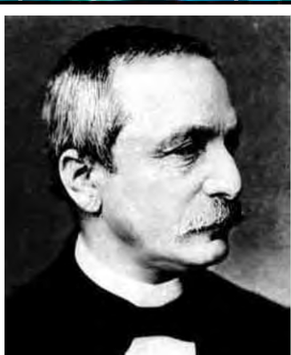
I continue with a variety of visual examples of high performance computing and communicating as part of

Experimental Inductive Mathematics

Our web site:

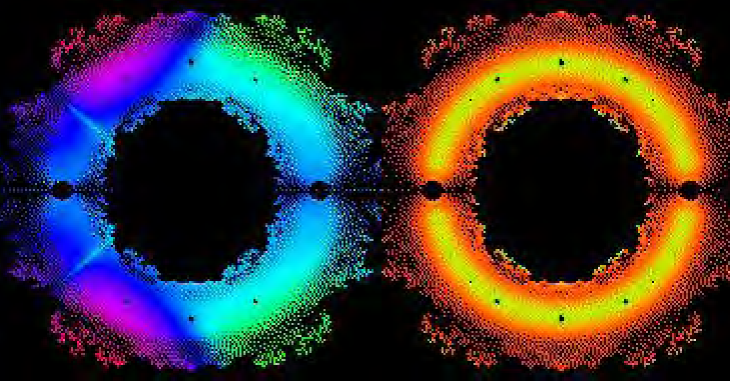
www.experimentalmath.info

contains all links and references



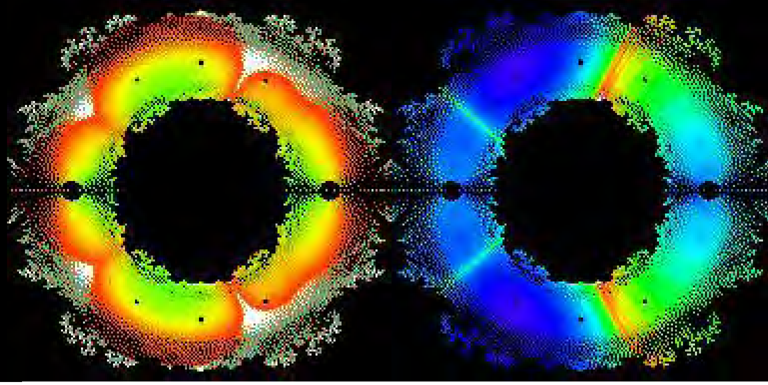
"Elsewhere Kronecker said ``In mathematics, I recognize true scientific value only in concrete mathematical truths, or to put it more pointedly, only in mathematical formulas." ... I would rather say ``computations" than ``formulas", but my view is essentially the same."

Harold Edwards, *Essays in Constructive Mathematics*, 2004



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

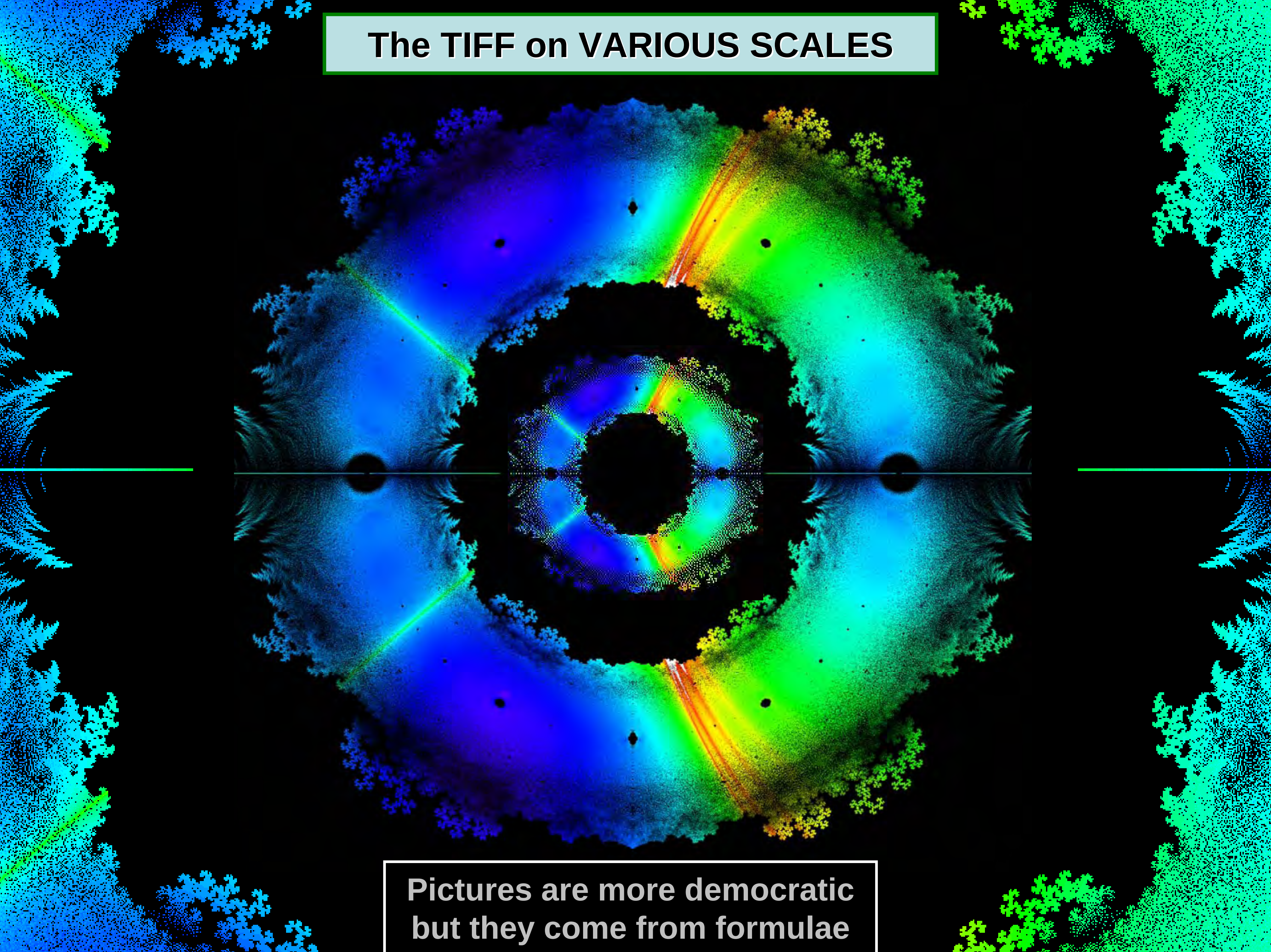
Coloration is by sensitivity of polynomials to slight variation around the values of the zeros. **The color scale represents a normalized sensitivity** to the range of values; red is insensitive to violet which is strongly sensitive.

- All zeros are pictured (at **3600 dpi**)
- Figure 1b is colored by their local density
- Figure 1d shows sensitivity relative to the $\mathbf{x^9}$ 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!"* Greg Chaitin, Interview, 2000.

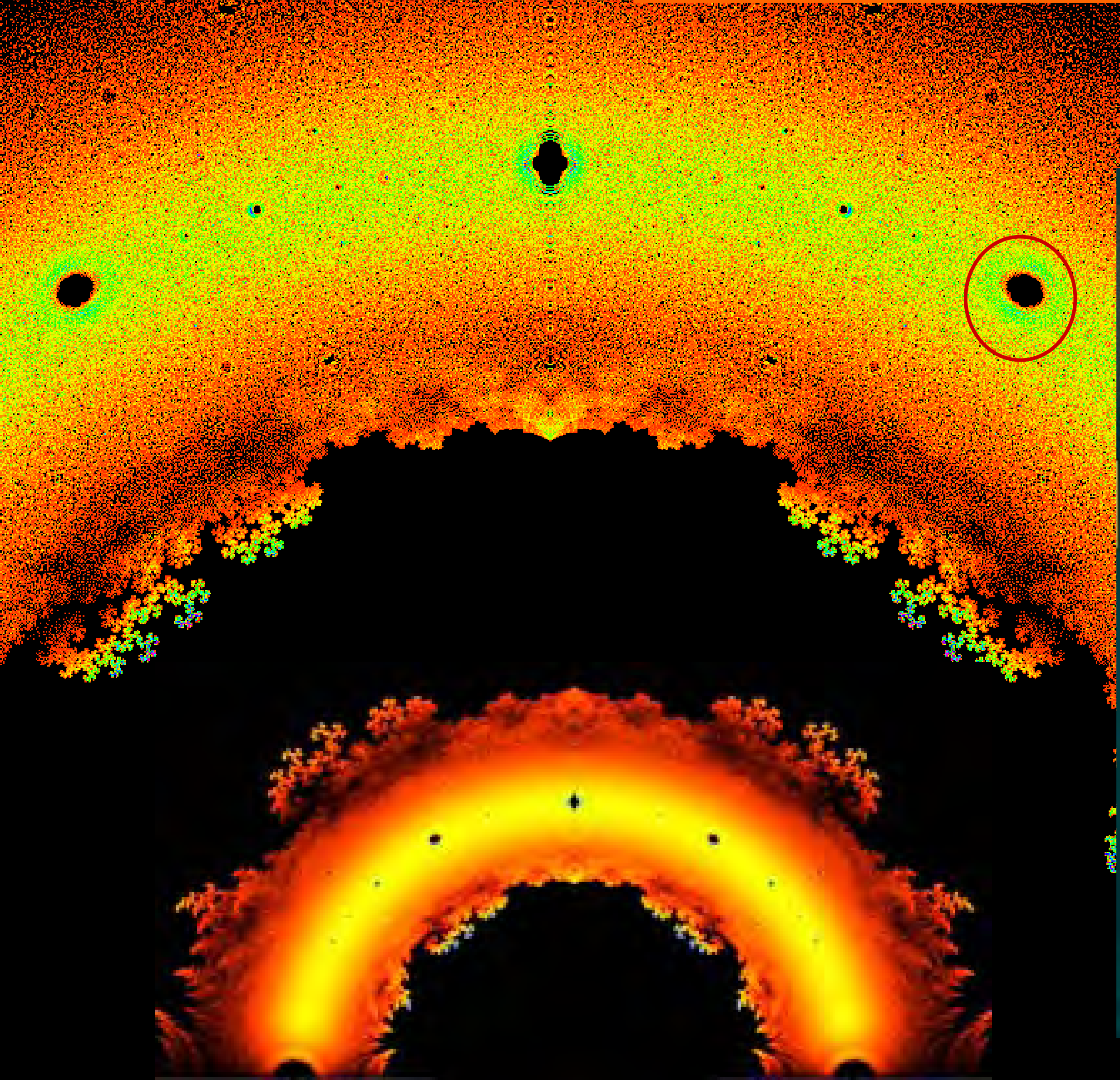
The TIFF on VARIOUS SCALES

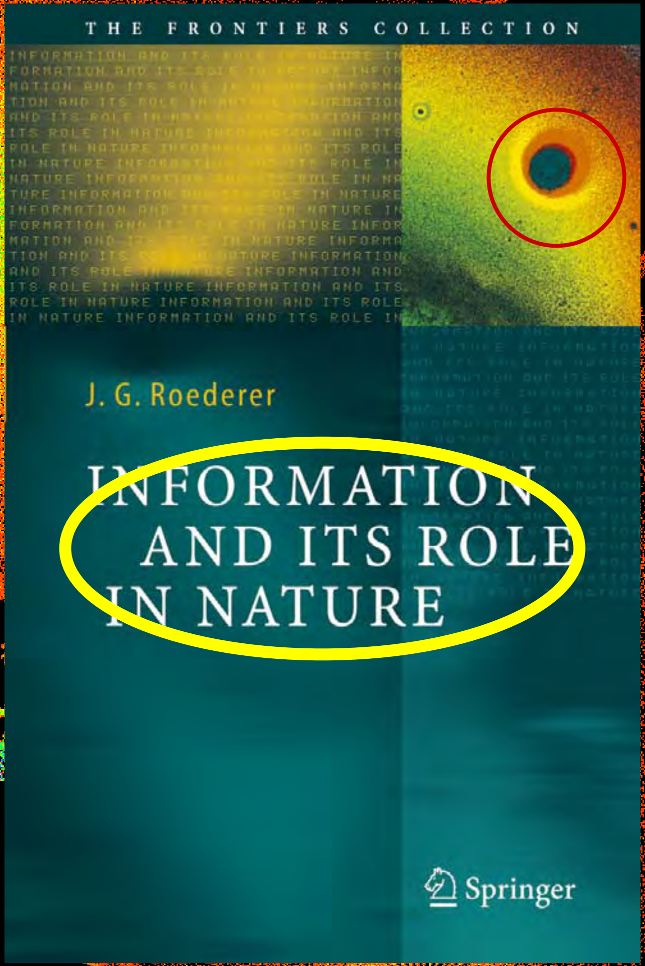


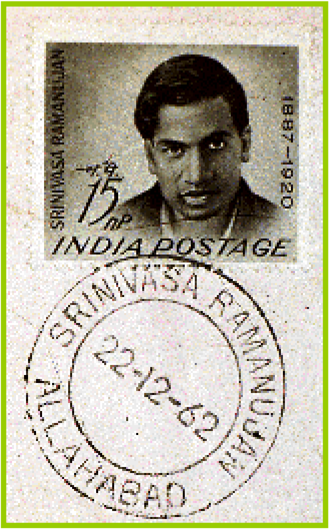
Pictures are more democratic
but they come from formulae

Roots in the most stable colouring

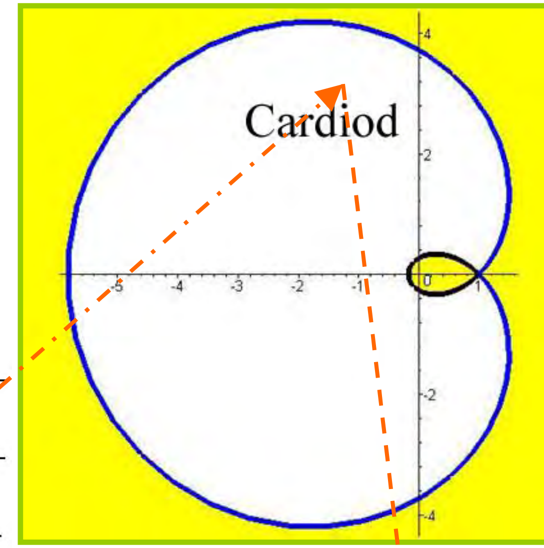
(The Sciences of the Artificial, Simons)







Ramanujan's Arithmetic-Geometric Continued fraction (CF)



$$R_\eta(a,b) = \cfrac{a}{\eta + \cfrac{b^2}{\eta + \cfrac{4a^2}{\eta + \cfrac{9b^2}{\eta + \ldots}}}}$$

For a,b>0 the CF satisfies a lovely symmetrization

$$\mathcal{R}_\eta\left(\frac{a+b}{2}, \sqrt{ab}\right) = \frac{\mathcal{R}_\eta(a,b) + \mathcal{R}_\eta(b,a)}{2}$$

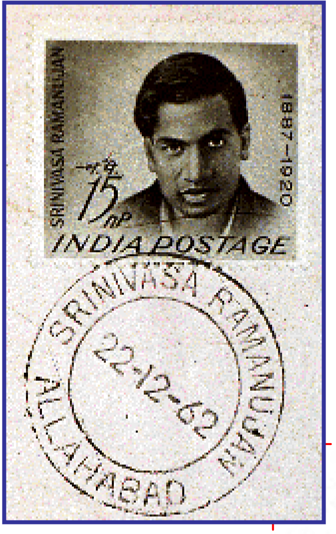
Computing directly was too hard; even 4 places of $\mathcal{R}_1(1,1) = \log 2$?

We wished to know for which a/b in C this all held

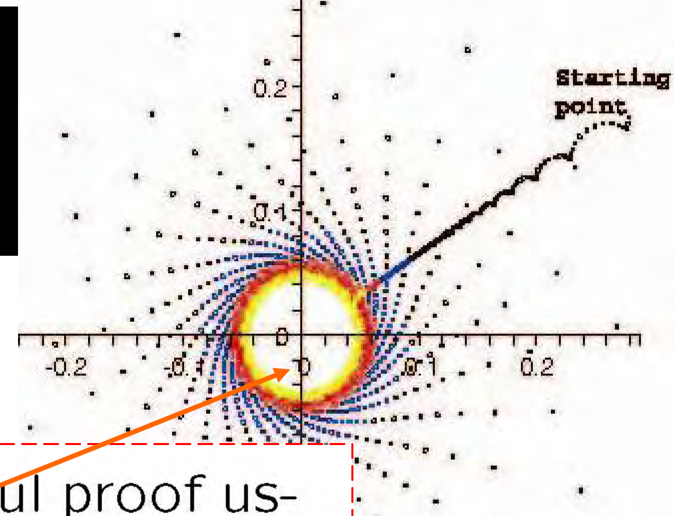
A scatterplot revealed a precise cardioid where r=a/b.

Which discovery it remained to prove?

$$\left|\frac{a+b}{2}\right| \geq \sqrt{|ab|}$$



Ramanujan's Arithmetic-Geometric Continued fraction



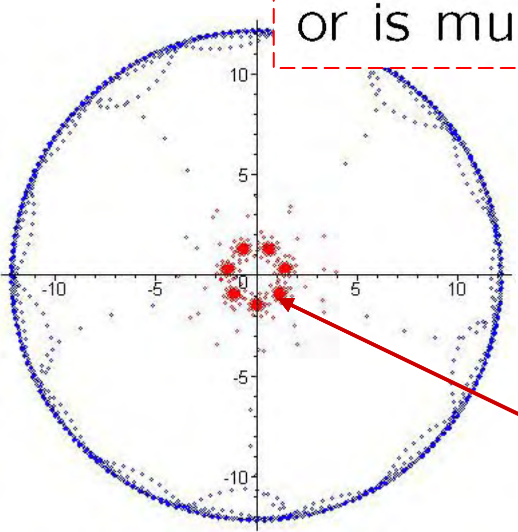
1. The Blackbox

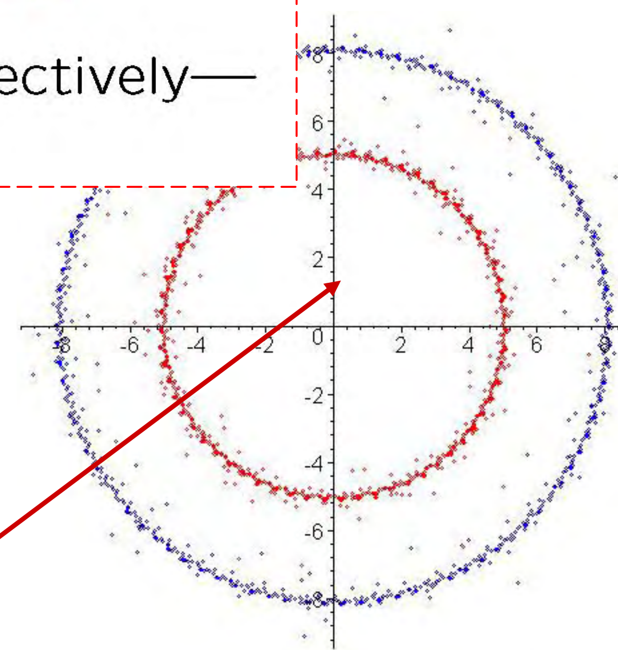
2. Seeing convergence

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

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

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

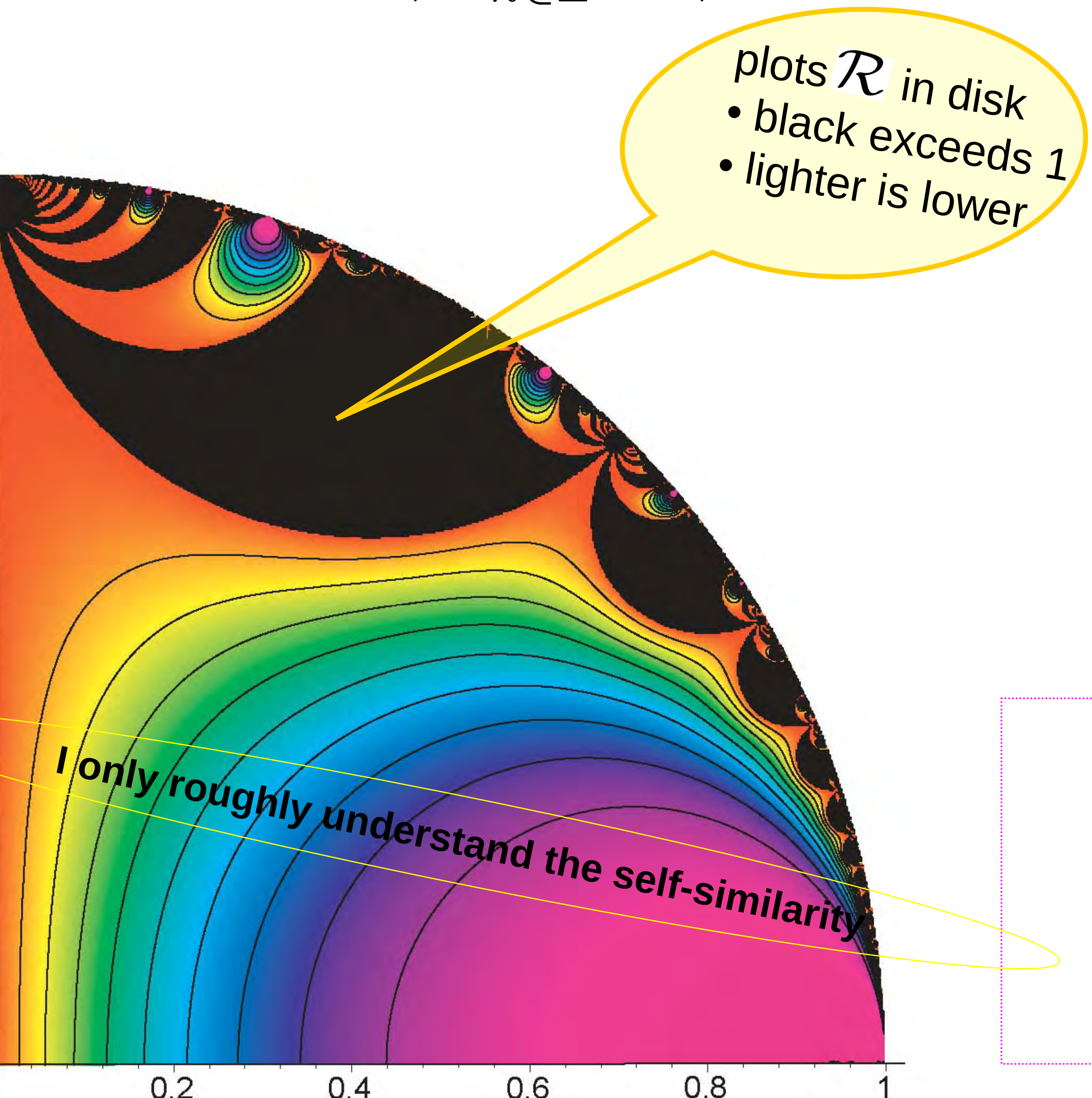


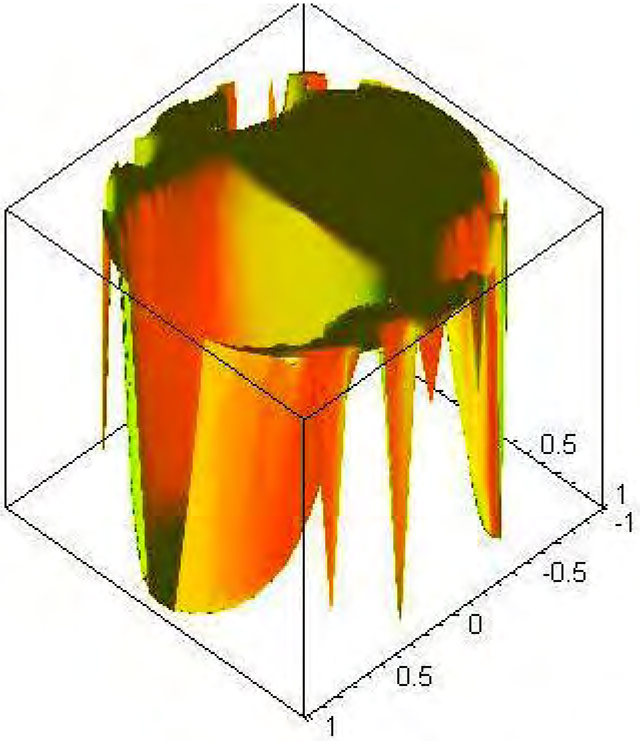


3. Attractors. *Normalizing* by $n^{1/2}$ three cases appear

$$\mathcal{R} = \frac{\left|\sum_{n\in\mathbf{Z}}(-1)^n q^{n^2}\right|}{\left|\sum_{n\in\mathbf{Z}} q^{n^2}\right|}$$

FRACTAL of a Modular Inequality



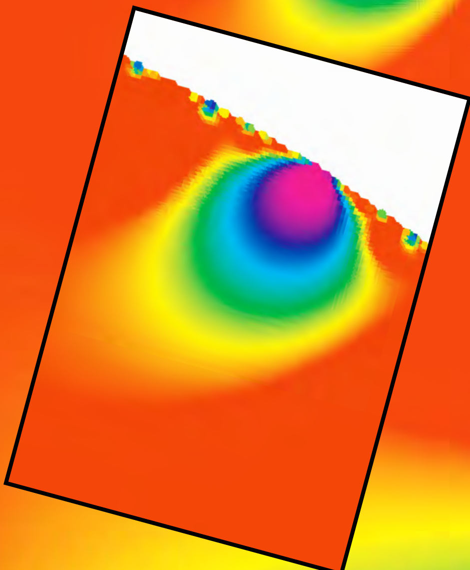


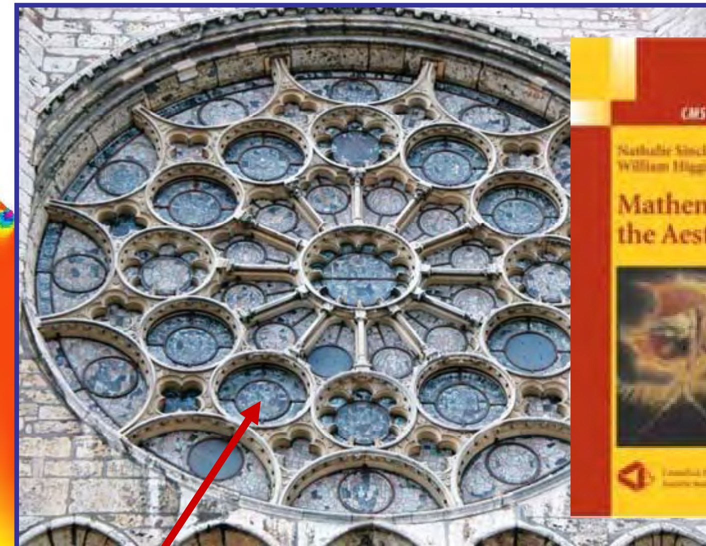
- ✓ related to Ramanujan's continued fraction
- ✓ took several hours to print
- ✓ Crandall/Apple has parallel print mode

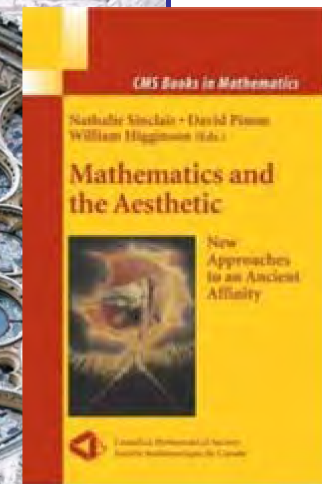
Mathematics and the aesthetic

Modern approaches to an ancient affinity

(CMS-Springer, 2006)







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.

B1. Visual Data Mining in Mathematics (old and new).

B2. Integer Relation Methods (and their numerics).

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

Sample 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(α) = 0 **OR**

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

Example (MAA, April 2005). Prove that

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

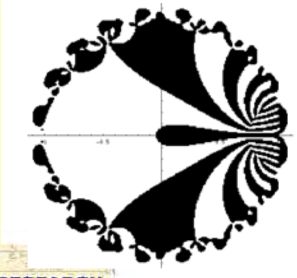
Proof. Purely **qualitative analysis** with partial fractions and arctans shows the integral is π β where β is algebraic of degree *much* less than **100 (actually 6)**, length *much* less than **100,000,000**.With **P(x)=x-1** (D=1,L=2, d=6, λ=?), this means *checking* the identity to **100** places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

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

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

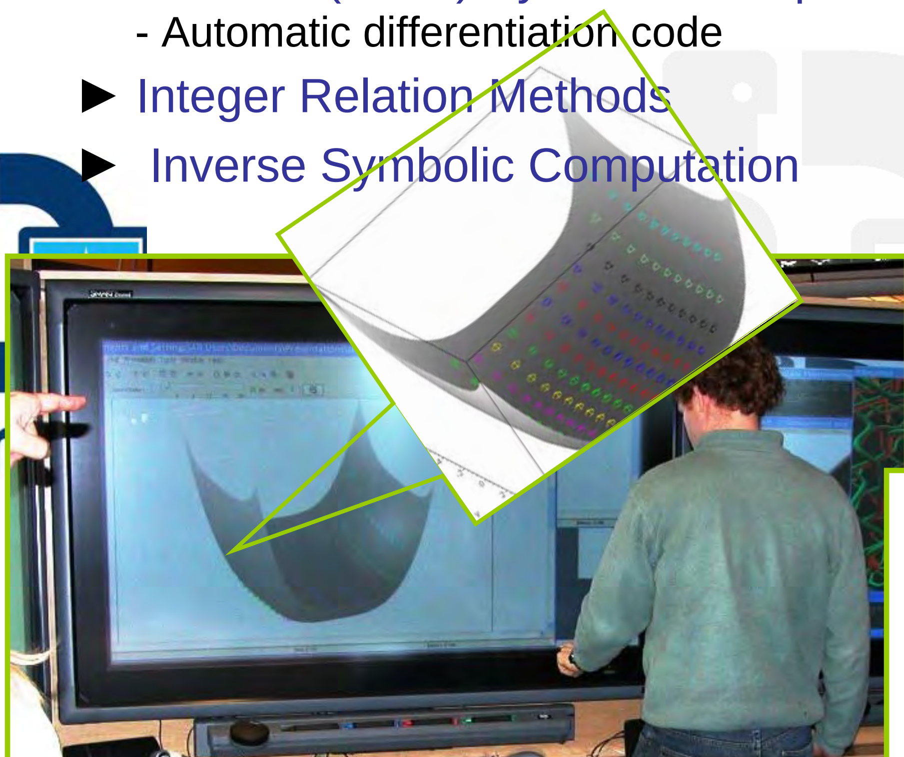
Drive

Hybrid Computation (Numeric and Symbolic)



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



Parallel derivative free optimization in ***Maple*** **(Glooscap 240 core)**

Other useful tools : Parallel Maple

- Sloane's online sequence database
- Salvy and Zimmerman's generating function package '*gfun*'
- Automatic identity proving: Wilf-Zeilberger method for hypergeometric functions

Greetings from the On-Line Encyclopedia of Integer Sequences!

Matches (up to a limit of 30) found for 1 2 3 6 11 23 47 106 235 :

[It may take a few minutes to search the whole database, depending on how many matches are found (the second and later look are faster)]

An Exemplary Database

ID Number: A000055 (Formerly M0791 and N0299)

URL: http://www.research.att.com/projects/OEIS?Anum=A000055

Sequence: 1,1,1,1,2,3,6,11,23,47,106,235,551,1301,3159,7741,19320, 48629,123867,317955,823065,2144505,5623756,14828074, 39299897,104636890,279793450,751065460,2023443032, 5469566585,14830871802,40330829030,109972410221

Name: Number of trees with n unlabeled nodes.

Comments: Also, number of unlabeled 2-gonal 2-trees with n 2-gons.

References
F. Bergeron, G. Labelle and P. Leroux, Combinatorial Species and Tree-Like Structures, Camb. 1998, p. 279.
N. L. Biggs et al., Graph Theory 1736-1936, Oxford, 1976, p. 49.
S. R. Finch, Mathematical Constants, Cambridge, 2003, pp. 295-316.
D. D. Grant, The stability index of graphs, pp. 29-52 of Combinatorial Mathematics (Proceedings 2nd Australian Conf.), Lect. Notes Math. 403, 1974.
F. Harary, Graph Theory. Addison-Wesley, Reading, MA, 1969, p. 232.
F. Harary and E. M. Palmer, Graphical Enumeration, Academic Press, NY, 1973, p. 58 and 244.
D. E. Knuth, Fundamental Algorithms, 3d Ed. 1997, pp. 386-88.
R. C. Read and R. J. Wilson, An Atlas of Graphs, Oxford, 1998.
J. Riordan, An Introduction to Combinatorial Analysis, Wiley, 1958, p. 138.

Links:
P. J. Cameron, Sequences realized by oligomorphic permutation groups J. Integ. Seqs. Vo
Steven Finch, Otter's Tree Enumeration Constants
E. M. 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. W. Weisstein, Link to a section of The World of Mathematics.
Index entries for sequences related to trees
Index entries for "core" sequences
G. Labelle, C. Lamathe and P. Leroux, Labeled and unlabeled enumeration of k-gonal 2-tr

Formula: G.f.: A(x) = 1 + T(x)-T^2(x)/2+T(x^2)/2, where T(x) = x + x^2 + 2*x^3 + ...

Integrated real time use

- moderated
- 120,000 entries
- grows daily
- AP book had 5,000

http://dlmf.nist.gov First 21C database

Digital Library of Mathematical Functions

Chapter AI. Airy & Related Functions
Properties

§AI.3. Graphs & Visualizations | §AI.5. Integral Representations

§AI.4. Maclaurin Series

For $z \in \mathbb{C}$

AI.4.1

$$\mathrm{Ai}(z) = \mathrm{Ai}(0)\left(1 + \frac{1}{3!}z^3 + \frac{1\cdot 4}{6!}z^6 + \frac{1\cdot 4\cdot 7}{9!}z^9 + \cdots\right) + \mathrm{Ai}'(0)\left(z + \frac{2}{4!}z^4 + \frac{2\cdot 5}{7!}z^7 + \frac{2\cdot 5\cdot 8}{10!}z^{10} + \cdots\right)$$

Symbols used:
AiryAi, cdots and z

A&S Ref:
10.4.2 (with 10.4.4 and 10.4.5)

Encodings:
LaTeX

Parsed:

```
AiryAi@(z) = AiryAi@(0) * (1 + (1 / 3!)
* z ^ 3 + ((1 cdot 4) / 6!) * z ^ 6 +
((1 cdot 4 cdot 7) / 9!) * z ^ 9 +
cdots) + (diffop@(AiryAi, 1))@(0) * (z +
(2 / 4!) * z ^ 4 + ((2 cdot 5) / 7!) * z
^ 7 + ((2 cdot 5 cdot 8) / 10!) * z ^ 10
+ cdots)
```

- **Formula level metadata**
- **Mathematical searching**
- **Accessible output**
- **Latex, PNG MathML**

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January 12, 2006

Supported by NIST National Institute of Standards and Technology and National Science Foundation Celebrating 50 Years

AI.4.2

$$\mathrm{Ai}'(z) = \mathrm{Ai}'(0)\left(1 + \frac{2}{3!}z^3 + \frac{2\cdot 5}{6!}z^6 + \frac{2\cdot 5\cdot 8}{9!}z^9 + \cdots\right) + \mathrm{Ai}(0)\left(\frac{1}{2!}z^2 + \frac{1\cdot 4}{5!}z^5 + \frac{1\cdot 4\cdot 7}{8!}z^8 + \cdots\right),$$

AI.4.3

$$\mathrm{Bi}(z) = \mathrm{Bi}(0)\left(1 + \frac{1}{3!}z^3 + \frac{1\cdot 4}{6!}z^6 + \frac{1\cdot 4\cdot 7}{9!}z^9 + \cdots\right) + \mathrm{Bi}'(0)\left(z + \frac{2}{4!}z^4 + \frac{2\cdot 5}{7!}z^7 + \frac{2\cdot 5\cdot 8}{10!}z^{10} + \cdots\right)$$

AI.4.4

$$\mathrm{Bi}'(z) = \mathrm{Bi}'(0)\left(1 + \frac{2}{3!}z^3 + \frac{2\cdot 5}{6!}z^6 + \frac{2\cdot 5\cdot 8}{9!}z^9 + \cdots\right) + \mathrm{Bi}(0)\left(\frac{1}{2!}z^2 + \frac{1\cdot 4}{5!}z^5 + \frac{1\cdot 4\cdot 7}{8!}z^8 + \cdots\right).$$

§AI.3. Graphs & Visualizations | §AI.5. Integral Representations

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:

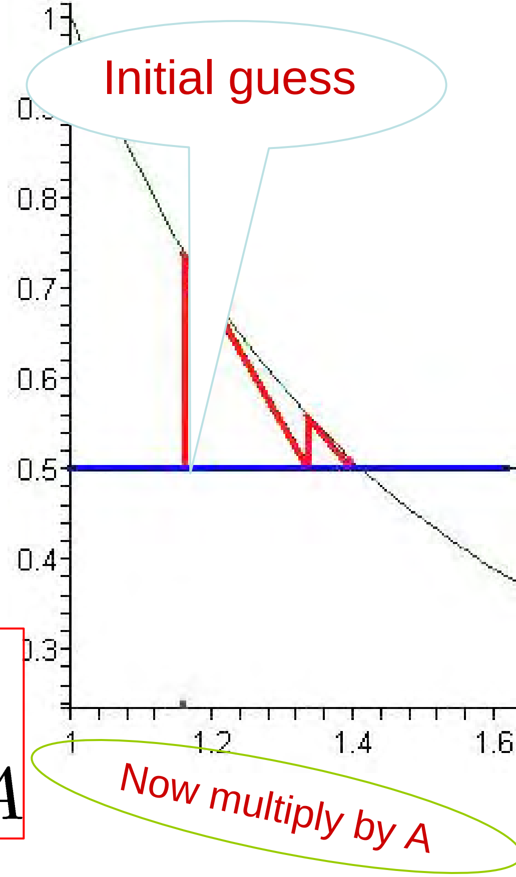
$$
\begin{aligned}
&\left(a + c \cdot 10^N\right) \times \left(b + d \cdot 10^N\right) \\
&= ab + (ad + bc) \cdot 10^N + cd \cdot 10^{2N} \\
&= ab + \underbrace{\{(a+c)(b+d) - ab - cd\}}_{\text{three multiplications}} \cdot 10^N + cd \cdot 10^{2N}
\end{aligned}
$$

Karatsuba replaces one 'times' by many 'plus'

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

$$x \hookleftarrow x - \frac{f(x)}{\frac{d}{dx}f(x)}$$

Newton's Method for Elementary Operations and Functions



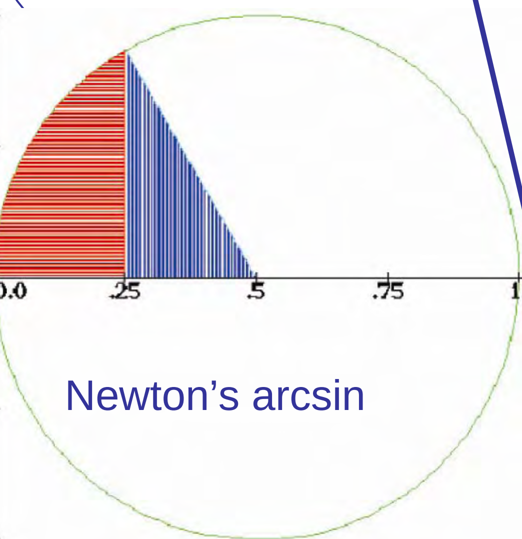
1. Doubles precision at each step
   Newton is **self correcting** and **quadratically convergent**
2. Consecutive **work needed**:

$$\text{'}\div = 4\times\text{'} : 1/x = A$$

$$\text{'}\sqrt{\cdot} = 6\times\text{'} : 1/x^2 = A$$

$$x \hookleftarrow x(2 - xA)$$

$$x \hookleftarrow 1/2\,x\left(3 - x^2 A\right)$$



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

Applied to Ising Integrals
(J. Phys. A, 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:

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

$C_{n,k}$ satisfies remarkable recurrences

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

Outline of HPMKM Talk

A. Communication, Collaboration and Computation.

B1. Visual Data Mining in Mathematics (old and new).

B2. Integer Relation Methods (and their numerics).

B3. Inverse Symbolic Computation.

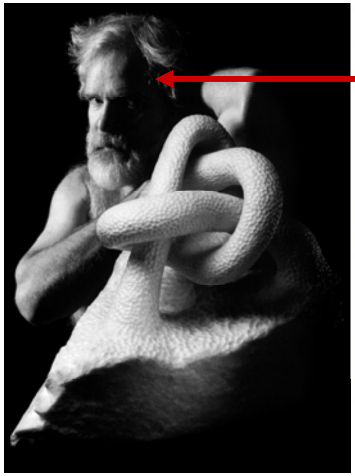
The talk ends when I do

The PSLQ Integer Relation Algorithm

Integer Relation Methods

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

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

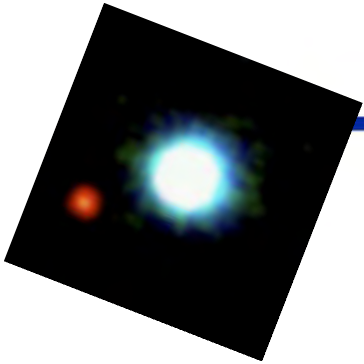


- At the present time, the PSLQ algorithm of mathematician-sculptor Helaman Ferguson is the best-known integer relation algorithm. **Science Oct 2006**
- PSLQ was named one of ten "algorithms of the century" by *Computing in Science and Engineering*.
- High precision arithmetic software is required: at least d 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

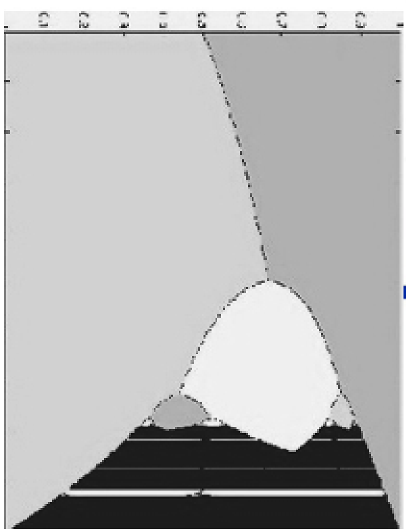
$B_3 = 3.54409035955\ldots$ is third bifurcation point of the logistic iteration of chaos theory:

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

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)

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

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

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

1

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

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

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

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?

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:

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

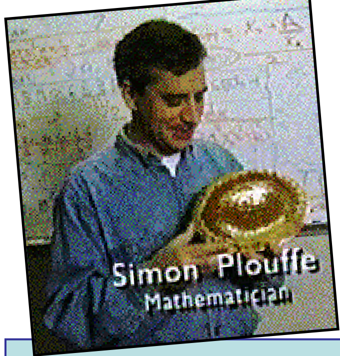
and execute:

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

which returns the certificate

```
          /     2                        \
          \11 n   + 1 + 6 n + k + 5 k n/ k
       - ---------------------------------
            3 (n - k + 1) (2 n + k + 1) n
```

This proves that summing $F(n,k)$ over k produces $r(n)$, as asserted.



PSLQ and Hex Digits of Pi

Finalist for the $100K Edge of Computation Prize won by David Deutsch (2005)

$$\log 2 = \sum_{n=1}^{\infty} \frac{1}{k\,2^k}$$

My brother made the observation that this log formula

Edge The Third Culture

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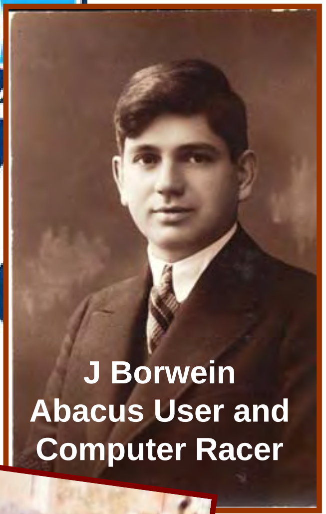
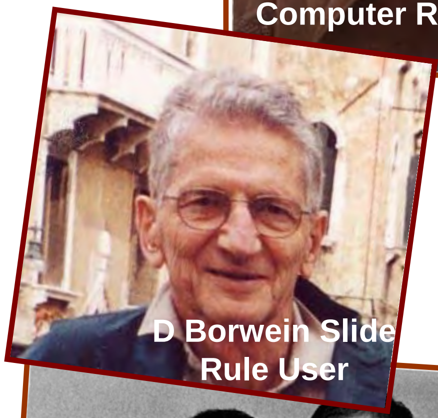
THE $100,000 EDGE OF COMPUTATION SCIENCE PRIZE

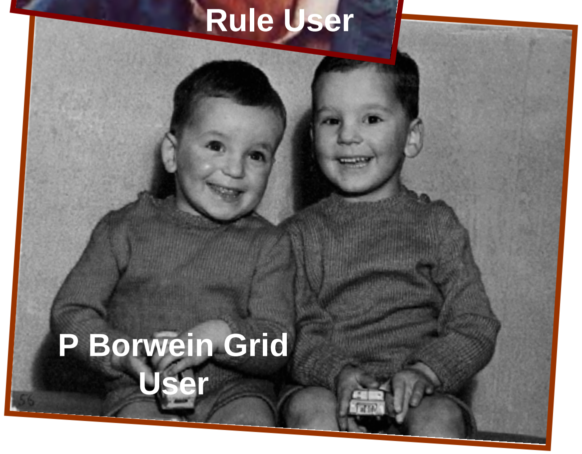
For individual scientific work, extending the computational idea, performed, published, or newly applied within the past ten years.

The Edge of Computation Science Prize, established by Edge Foundation, Inc., is a $100,000 prize initiated and funded by science philanthropist Jeffrey Epstein.

The pre-designed Algorithm ran the next day







ALGORITHMIC PROPERTIES

(1) produces a modest-length string hex or binary digits of π, beginning at an arbitrary position, using no prior bits;

Now built into some compilers!

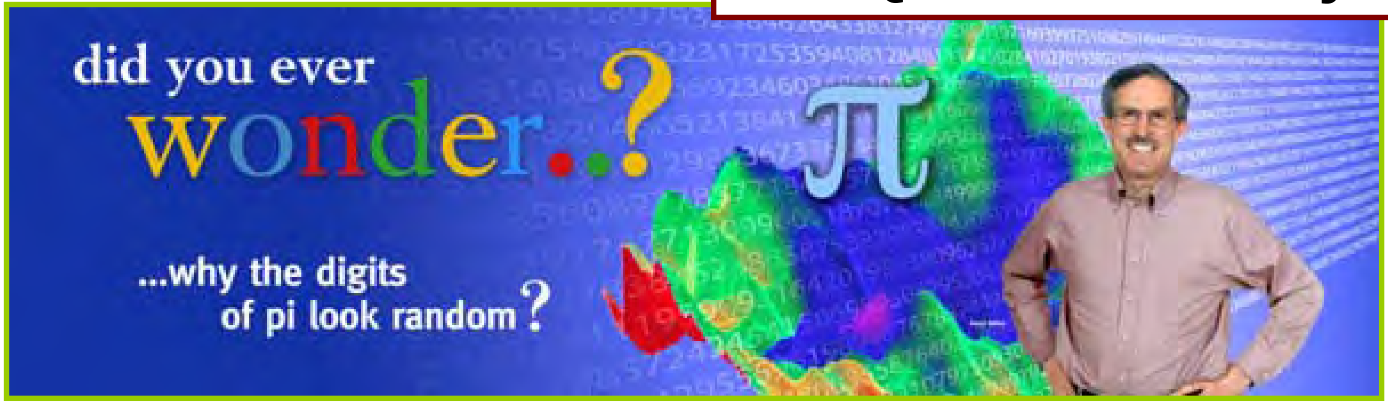
(2) is implementable on any modern computer;

(3) requires no multiple precision software;

(4) requires very little memory; and

(5) has a computational cost growing only slightly faster than the digit position.

PSLQ and Normality of Digits



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]

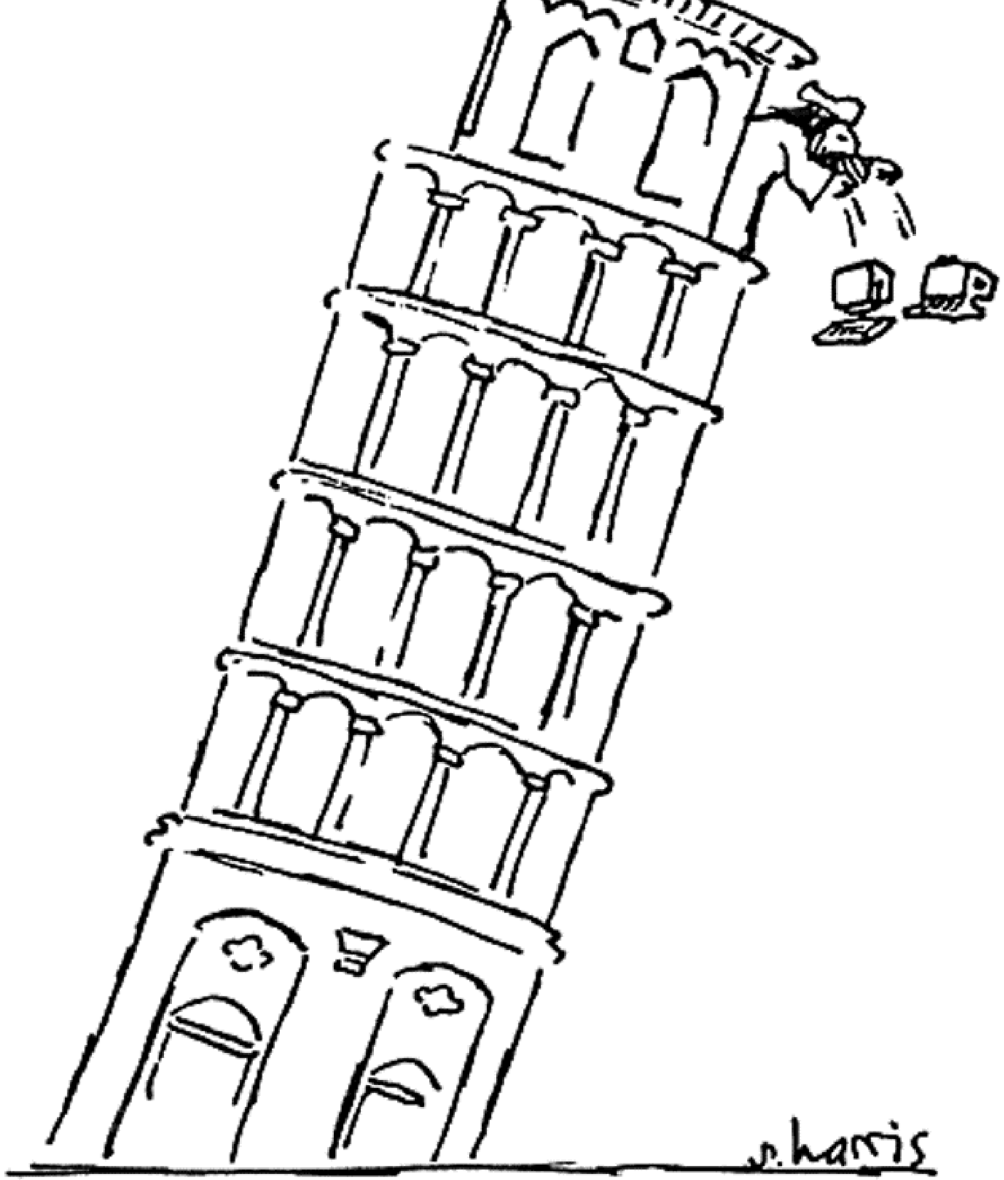
$$x_n = \left\{ 16x_{n-1} + \frac{120n^2 - 89n + 16}{512n^4 - 1024n^3 + 712n^2 - 206n + 21} \right\}$$

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.

B1. Visual Data Mining in Mathematics (old and new).

B2. Integer Relation Methods (and their numerics).

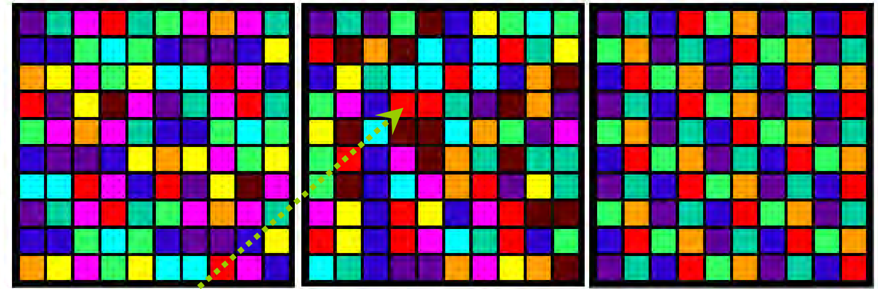
B3. Inverse Symbolic Computation.

The talk ends when I do

"On the Internet, nobody knows you're a dog."

A Colour and an Inverse Calculator (1995 & 2007)

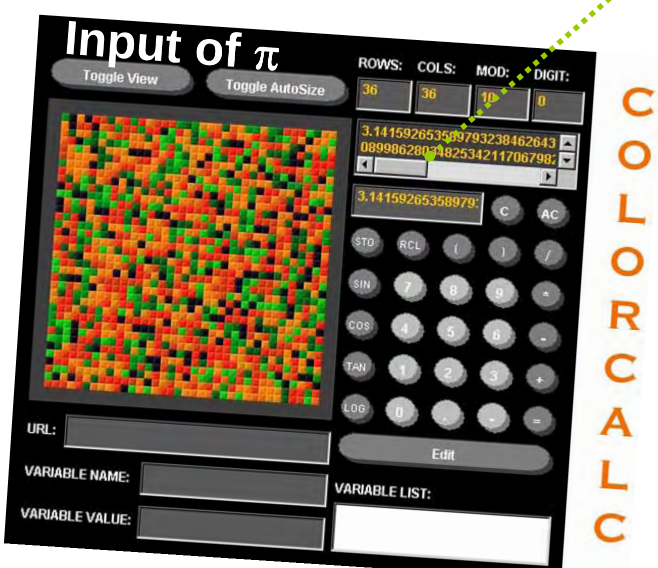
Inverse Symbolic Computation



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

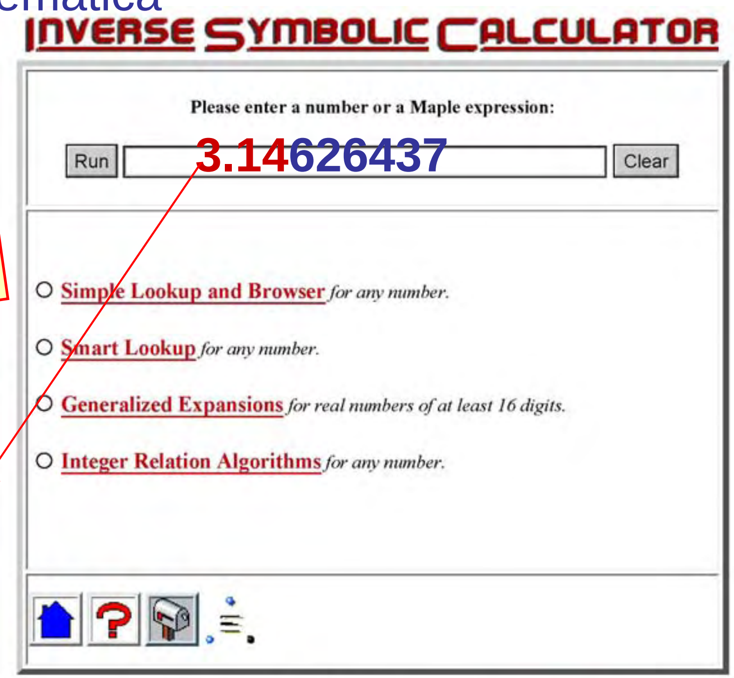
Inferring mathematical structure from numerical data

- 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.))

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



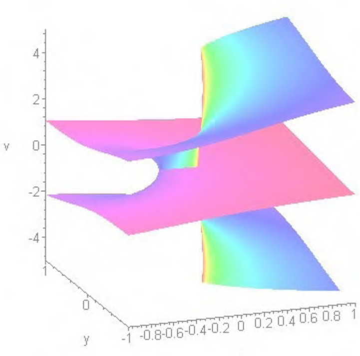
Expressions that are **not** numeric like ln(Pi*sqrt(2)) are evaluated in Maple in symbolic form first, followed by a floating point evaluation followed by a lookup.

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



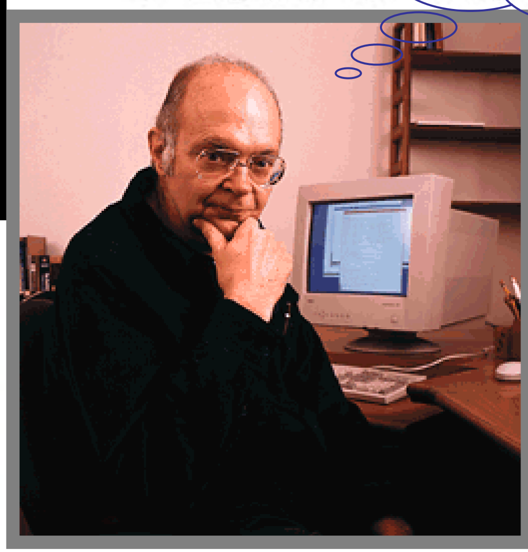
W's **Riemann** surface

Donald Knuth* asked for a closed form evaluation of:

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

"instrumentality"

- **2000 CE.** It is easy to compute 20 or 200 digits



ISC is shown on next slide

lookup' facility in the *Inverse Sym-*

lator† rapidly returns

$$4069508727655 \approx \frac{2}{3} + \frac{\zeta(1/2)}{\sqrt{2\,\pi}}.$$

We thus have a prediction which *Maple* 9.5 on a laptop confirms to 100 places in under 6 seconds and to 500 in 40 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.

Quadrature I. Hyperbolic Knots

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

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]

We have certain knowledge without proof

Extreme Quadrature … 20,000 Digits (50 Certified) on 1024 CPUs

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

Perko knots 10_{162} and 10_{163} agree: a dynamic proof

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

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

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)

Quadrature II. Ising Susceptibility Integrals

Bailey, Crandall and I recently studied:

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

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

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

D_4 is a remarkable 1977 result due to McCoy--Tracy--Wu

Computer Algebra Systems can (with help) find the first 3

An Extreme Ising Quadrature

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

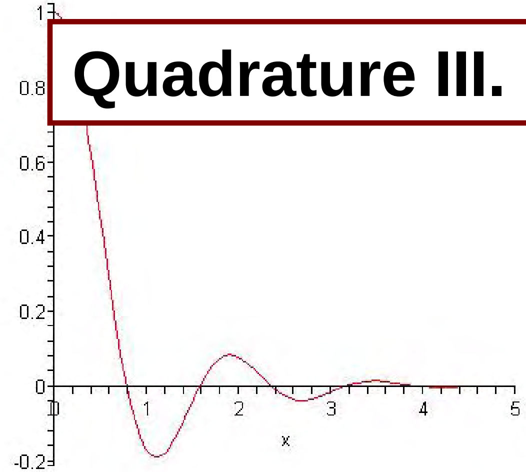
✓ We are able to reduce D_5 to a horrifying several-page-long 3-D symbolic integral !

✓**A 256 cpu 'tanh-sinh' computation at LBNL** A FIRST: data for all

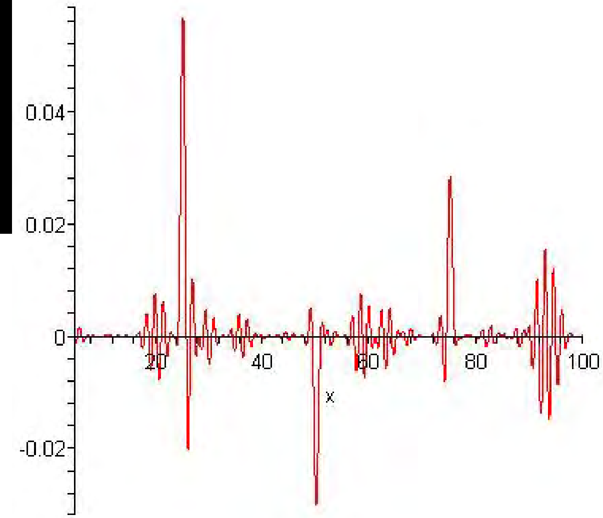
18.2 hours on "Bassi", an IBM Power5 system:

0.002484605762340315479950509153909749635060677642487516158707692161822137856915435753792689948724512018706872110639252051186206994499754226565626467085382841245001166822300045457032687697384896151982479613035525258515107154386381136961749224298557807628042894777027871092119811160634063125413603859840198280786401869307268109885482303788788487583058351257855236419969486914631409112736309460524093400887162838706436421861204509029973356634113727612202408834546315017113540844197840922456685046081844 68...

Quadrature III. Pi/8?



A numerically challenging integral tamed



$$\int_0^\infty \cos(2x) \prod_{n=1}^{\infty} \cos\left(\frac{x}{n}\right) dx \stackrel{?}{=} \frac{\pi}{8}.$$

Now **π/8** equals

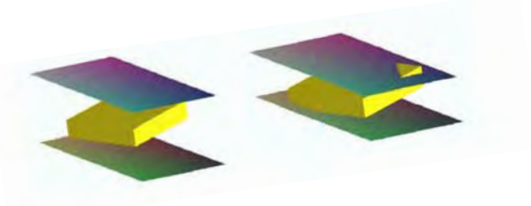
$0.392699081698724154807830422909937860524645434$

while the **integral** is

$0.392699081698724154807830422909937860524646174 9$

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

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



Before and After

REFERENCES


Enigma

J.M. Borwein and D.H. Bailey, *Mathematics by Experiment: Plausible Reasoning in the 21st Century* A.K. Peters, 2003. and R. Girgensohn, *Experimentation in Mathematics: Computational Paths to Discovery,* A.K. Peters, 2004.

[Active CDs 2006]

D.H. Bailey and J.M Borwein, "Experimental Mathematics: Examples, Methods and Implications," *Notices Amer. Math. Soc.*, **52** No. 5 (2005), 502-514.

J. Borwein, D. Bailey, N. Calkin, R. Girgensohn, R. Luke, and V. Moll, Experimental Mathematics in Action, A.K. Peters, 2007

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

- J. Hadamard quoted at length in E. Borel, *Lecons sur la theorie des fonctions*, 1928.


THEORIES
PROOFS
S. Harris