

# Mathematics by Experiment:

## Plausible Reasoning in the 21st Century



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## Experimental Mathematics Lecture

October 2004

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 Gödel, 1951)

URL: [www.expmath.info](http://www.expmath.info)



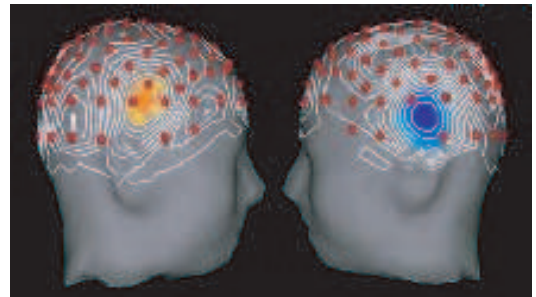
**AK Peters** 2004

Talk Revised: 04-10-04

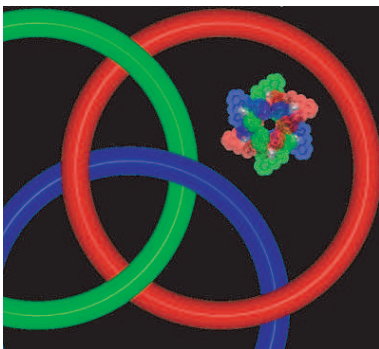
## MY INTENTIONS IN THIS TALK

- to discuss Experimental Methodology\*
  - its philosophy
  - its practice
  - using concrete amusing (I hope) examples

Insight taking place



Molecular Borromean Rings



- and then to
- review its past
  - describe its present
  - predict its future

- Thereby, to persuade you that traditional accounting of mathematical learning and research is largely an ahistorical caricature<sup>†</sup>

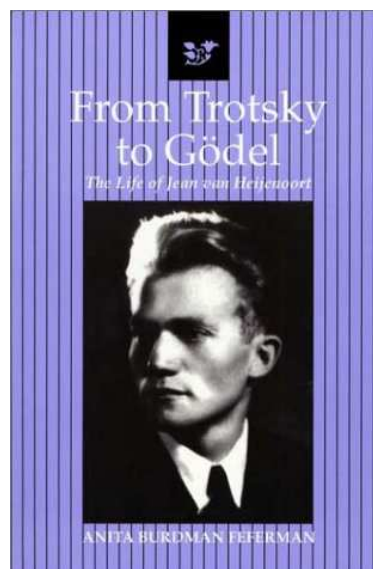
\*Bailey, Moll and I invite you to the 2nd [Experimental Mathematics Workshop](#) at Tulane, Spring 2005

<sup>†</sup>Online is a superset of this talk

## FROM TROTSKY to GÖDEL: a **LIFE**

"By 1948, the Marxist-Leninist ideas about the proletariat and its political capacity seemed more and more to me to disagree with reality ... I pondered my doubts, and for several years the study of mathematics was all that allowed me to preserve my inner equilibrium. Bolshevik ideology was, for me, in ruins. I had to build another life."

Jean Van Heijenoort (1913-1986) *With Trotsky in Exile*, in Anita Feferman's *From Trotsky to Gödel*



## IT'S OBVIOUS

**Aspray:** Since you both [Kleene and Rosser] had close associations with Church, I was wondering if you could tell me something about him. What was his wider mathematical training and interests? What were his research habits? I understood he kept rather unusual working hours. How was he as a lecturer? As a thesis director?

**Rosser:** In his lectures he was painstakingly careful. There was a story that went the rounds. *If Church said it's obvious, then everybody saw it a half hour ago. If Weyl says it's obvious, von Neumann can prove it. If Lefschetz says it's obvious, it's false.* \*

\*One of several versions in *The Princeton Mathematics Community in the 1930s*. This one in Transcript Number 23 (**PMC23**)

## THE EVIL of BOURBAKI

“There is a story told of the mathematician Claude Chevalley (1909–84), who, as a true Bourbaki, was extremely opposed to the use of images in geometric reasoning.



He is said to have been giving a very abstract and algebraic lecture when he got stuck. After a moment of pondering, he turned to the blackboard, and, trying to hide what he was doing, drew a little diagram, looked at it for a moment, then quickly erased it, and turned back to the audience and proceeded with the lecture. ...

... The computer offers those less expert, and less stubborn than Chevalley, access to the kinds of images that could only be imagined in the heads of the most gifted mathematicians, ...” (Nathalie Sinclair<sup>a</sup>)

<sup>a</sup>Chapter in *Making the Connection: Research and Practice in Undergraduate Mathematics*, MAA Notes, 2004 in Press.

**Abstract.** I shall talk generally about experimental and heuristic mathematics, and give accessible, primarily visual and symbolic, examples.

The emergence of powerful mathematical computing environments like *Maple* and *Matlab*, the growing availability of correspondingly powerful (*multi-processor*) computers and the pervasive presence of the internet allow for research mathematicians, students and teachers, to proceed heuristically and ‘quasi-inductively’.

We may increasingly use symbolic and numeric computation visualization tools, simulation and data mining. Likewise, an aesthetic appreciation of mathematics may be provided to a much broader audience.

Many of the benefits of computation are accessible through low-end ‘electronic blackboard’ versions of experimental mathematics. This also permits livelier classes, more realistic examples, and more collaborative learning. Moreover, the distinction between computing (HPC) and communicating (HPN) is increasingly moot.

**The unique features of the discipline make this both more problematic and more challenging.**

- For example, there is still no truly satisfactory way of displaying mathematical notation on the web;
- and we care more about the reliability of our literature than does any other science.

**The traditional central role of proof in mathematics is arguably under siege.**

Limned by examples, I intend to ask:

- ★ What constitutes secure mathematical knowledge?
  
- ★ When is computation convincing? Are humans less fallible?
  - What tools are available? What methodologies?
  
  - What about the 'law of the small numbers'?
  
  - Who cares for certainty? What is the role of proof?
  
- ★ How is mathematics actually done? How should it be?



And I shall offer some personal conclusions.

- ▶ Many of the more sophisticated examples originate in the boundary between mathematical physics and number theory and involve the  $\zeta$ -function,  $\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n}$ , and its relatives.

They often rely on the sophisticated use of *Integer Relations Algorithms* — recently ranked among the ‘top ten’ algorithms of the century.

- **Integer Relation methods** were first discovered by our colleague **Helaman Ferguson** the mathematical sculptor.

See [www.cecm.sfu.ca/projects/IntegerRelations/](http://www.cecm.sfu.ca/projects/IntegerRelations/)

## SOME SELF PROMOTION

- Experimental Mathematics is being discussed widely

MATH

### A Digital Slice of Pi

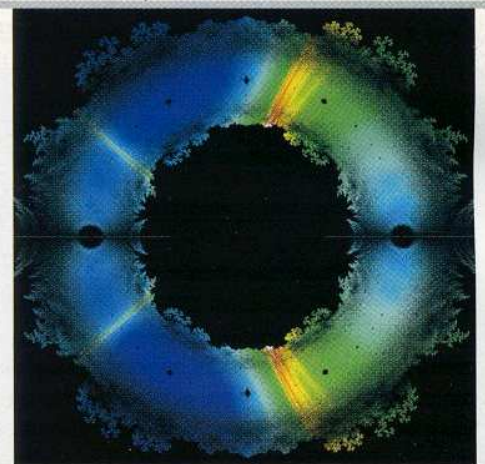
THE NEW WAY TO DO PURE MATH: EXPERIMENTALLY BY W. WAYT GIBBS

“One of the greatest ironies of the information technology revolution is that while the computer was conceived and born in the field of pure mathematics, through the genius of giants such as John von Neumann and Alan Turing, until recently this marvelous technology had only a minor impact within the field that gave it birth.” So begins *Experimentation in Mathematics*, a book by Jonathan M. Borwein and David H. Bailey due out in September that documents how all that has begun to change. Computers, once looked on by mathematical researchers with disdain as mere calculators, have gained enough power to enable an entirely new way to make fundamental discoveries: by running experiments and observing what happens.

The first clear evidence of this shift emerged in 1996. Bailey, who is chief technologist at the National Energy Research Sci-

entific Computing Center in Berkeley, Calif., and several colleagues developed a computer program that could uncover integer relations among long chains of real numbers. It was a problem that had long vexed mathematicians. Euclid discovered the first integer relation scheme—a way to work out the greatest common divisor of any two integers—around 300 B.C. But it wasn’t until 1977 that Helaman Ferguson and Rodney W. Forcade at last found a method to detect relations among an arbitrarily large set of numbers. Building on that work, in 1995 Bailey’s group turned its computers loose on some of the fundamental constants of math, such as log 2 and pi.

To the researchers’ great surprise, after months of calculations the machines came up with novel formulas for these and other nat-



**COMPUTER RENDERINGS** of mathematical constructs can reveal hidden structure. The bands of color that appear in this plot of all solutions to a certain class of polynomials [specifically, those of the form  $\pm 1 \pm x \pm x^2 \pm x^3 \pm \dots \pm x^n = 0$ , up to  $n = 18$ ] have yet to be explained by conventional analysis.

www.sciam.com

SCIENTIFIC AMERICAN 23

From Scientific American, May 2003

# MATH LAB

## Computer experiments are transforming mathematics

BY ERICA KLARREICH

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

"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.

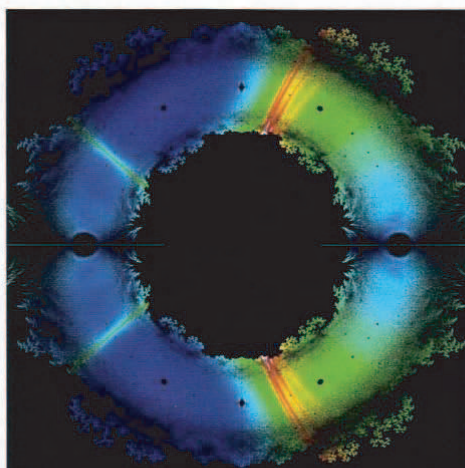
For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

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."

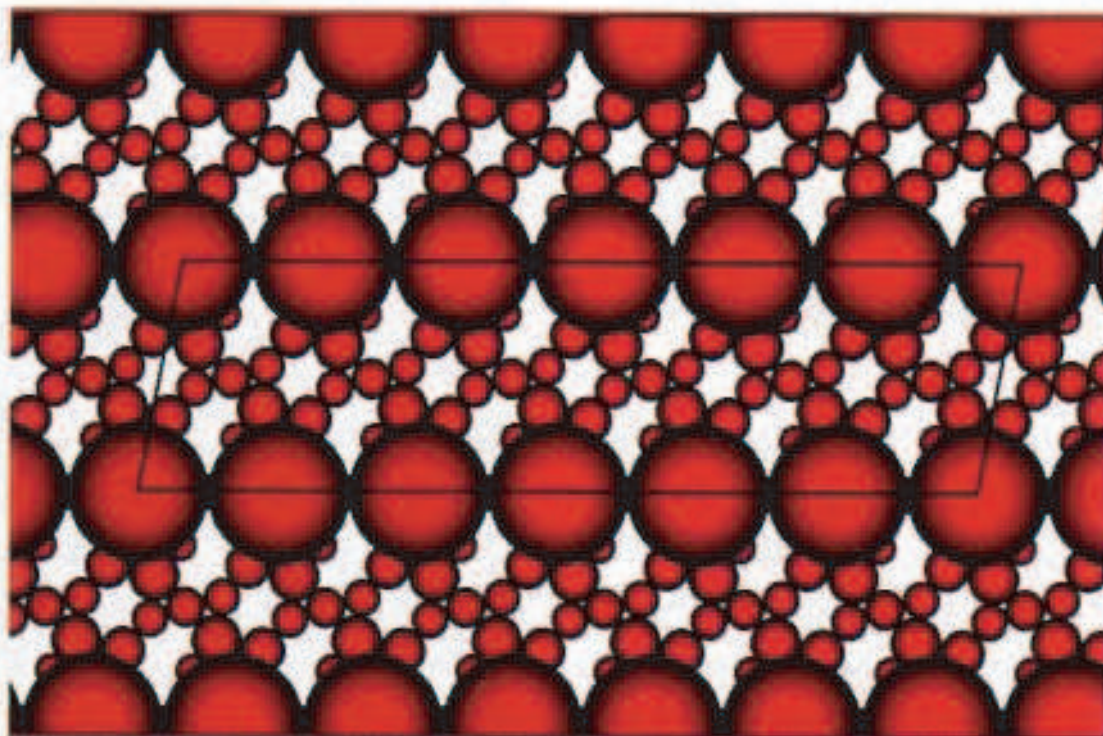
In the case of the prime number theorem, Gauss later refined his conjecture but never did figure out how to prove it. It took more than a century for mathematicians to come up with a proof.

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-



**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.

From Science News April 2004



**STRAIGHT CIRCLES** — When mathematicians Colin Adams and Eric Schoenfeld created this image while playing with the computer program Snappea last year, they were stunned to see perfectly straight chains of spheres. The observation led them to an unexpected discovery about knots.

Bailey and Jonathan Borwein advance the controversial thesis that mathematics should move toward a more empirical approach. In it, formal proof would not be the only acceptable way to establish mathematical knowledge.

Mathematicians, Bailey and Borwein argue, should be free to work more like other scientists do, developing hypotheses through experimentation and then testing them in further experiments. Formal proof is still the ideal, they say, but it is not the only path to mathematical truth.


“When I started school, I thought mathematics was about proofs, but now I think it’s about having secure mathematical knowledge,” Borwein says. “We claim that’s not the same thing.”

Bailey and Borwein point out that mathematical proofs can run to hundreds of pages and require such specialized knowledge that only a few people are capable of reading and judging them.

“We feel that in many cases, computations constitute very strong evidence, evidence that is at least as compelling as some of the more complex formal proofs in the literature,” Bailey and Borwein say in *Mathematics by Experiment*.

“One thing that’s happening is you can discover many more things than you can explain.”

— JONATHAN BORWEIN  
DALHOUSIE UNIVERSITY



## FINDING THINGS or PROVING THINGS

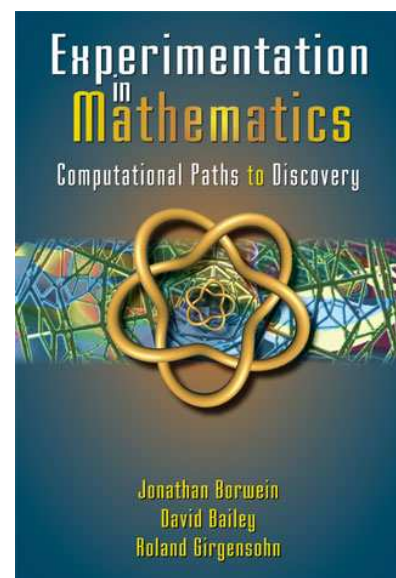
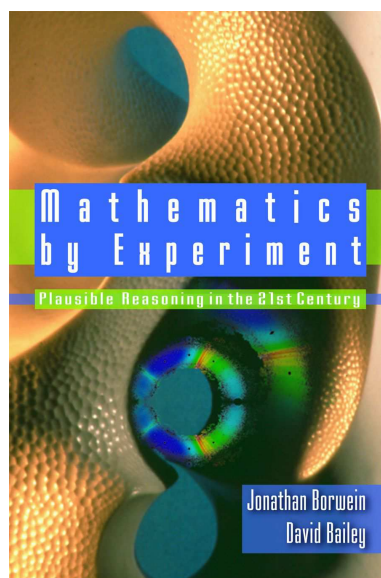
Consider the following two *Euler sum identities* both discovered heuristically.

- Both merit quite firm belief—more so than many proofs.

**Why?**

- Only the first warrants significant effort for its proof.

**Why** and **Why Not?**



## I. A MULTIPLE ZETA VALUE

*Euler sums* or *MZVs* are a wonderful generalization of the classical  $\zeta$  function.

For natural numbers

$$\zeta(i_1, i_2, \dots, i_k) := \sum_{n_1 > n_2 > \dots > n_k > 0} \frac{1}{n_1^{i_1} n_2^{i_2} \dots n_k^{i_k}}$$

◇ Thus  $\zeta(a) = \sum_{n \geq 1} n^{-a}$  is as before and

$$\zeta(a, b) = \sum_{n=1}^{\infty} \frac{1 + \frac{1}{2^b} + \dots + \frac{1}{(n-1)^b}}{n^a}$$

✓  $k$  is the sum's *depth* and  $i_1 + i_2 + \dots + i_k$  is its *weight*.

- This clearly extends to alternating and character sums.

- MZV's satisfy many striking identities, of which the simplest are

$$\zeta(2, 1) = \zeta(3) \quad 4\zeta(3, 1) = \zeta(4).$$

- MZV's have recently found interesting interpretations in high energy physics, knot theory, combinatorics ...
- ✓ Euler found and partially proved theorems on **reducibility** of depth 2 to depth 1  $\zeta$ 's
- $\zeta(6, 2)$  is the lowest weight **'irreducible'**.
- ✓ High precision *fast  $\zeta$ -convolution* (see *EZ-Face/Java*) allows use of integer relation methods and leads to important dimensional (reducibility) conjectures and amazing identities.



**A STRIKING CONJECTURE** open for all  $n > 2$  is:

$$8^n \zeta(\{-2, 1\}_n) \stackrel{?}{=} \zeta(\{2, 1\}_n),$$

There is abundant evidence amassed since it was found in 1996.\* For example, very recently Petr Lisonek checked the first 85 cases to 1000 places in about 41 HP hours with only the *expected error*. And  $N=163$  in ten hours.

- This is the *only* identification of its type of an Euler sum with a distinct MZV.
- Can even just the case  $n = 2$  be proven *symbolically* as is the case for  $n = 1$ ?

\*Equivalently that the functions

$$L_{-2,1}(1, 2t) = L_{2,1}(1, t) \quad (= L_3(1, t)),$$

defined later agree for small  $t$ .

## II. A CHARACTER EULER SUM

Let

$$[2b, -3](s, t) := \sum_{n>m>0} \frac{(-1)^{n-1} \chi_3(m)}{n^s m^t},$$

where  $\chi_3$  is the character modulo 3. Then for  $N = 0, 1, 2, \dots$

$$\begin{aligned} & [2b, -3](2N + 1, 1) \\ &= \frac{L_{-3}(2N + 2)}{4^{1+N}} - \frac{1 + 4^{-N}}{2} L_{-3}(2N + 1) \log(3) \\ &+ \sum_{k=1}^N \frac{1 - 3^{-2N+2k}}{2} L_{-3}(2N - 2k + 2) \alpha(2k) \\ &- \sum_{k=1}^N \frac{1 - 9^{-k}}{1 - 4^{-k}} \frac{1 + 4^{-N+k}}{2} L_{-3}(2N - 2k + 1) \alpha(2k + 1) \\ &- 2L_{-3}(1) \alpha(2N + 1). \end{aligned}$$

✓ Here  $\alpha$  is the *alternating zeta function* and  $L_{-3}$  is the *primitive L-series modulo 3*.

★ One first **evaluates** such sums as integrals

## DICTIONARIES ARE LIKE TIMEPIECES

- ▶ Samuel Johnson observed of watches that “the best do not run true, and the worst are better than none.” The same is true of tables and databases. Michael Berry “would give up Shakespeare in favor of Prudnikov, Brychkov and Marichev.”
- That excellent compendium contains

$$(1) \quad \sum_{k=1}^{\infty} \sum_{l=1}^{\infty} \frac{1}{k^2 (k^2 - kl + l^2)} = \frac{\pi^{\alpha} \sqrt{3}}{30},$$

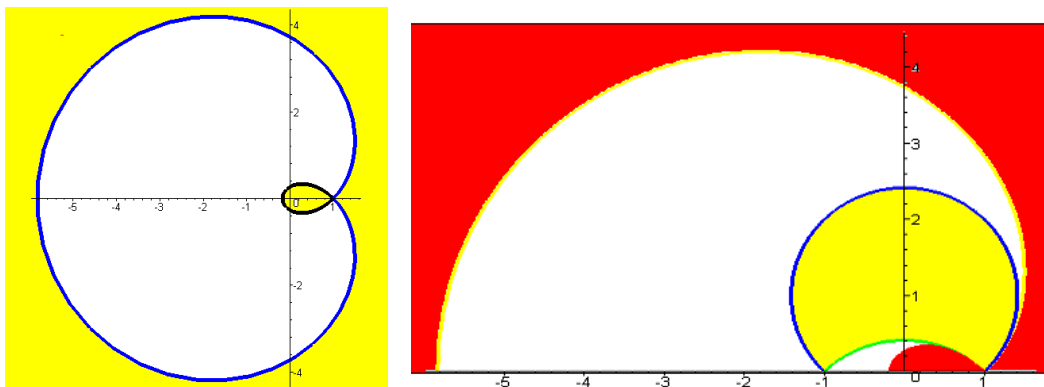
where the “ $\alpha$ ” is *probably* “4” [volume 1, entry 9, page 750].

- ★ Integer relation methods suggest that **no reasonable value of  $\alpha$  works.**

What is intended in (1)?

## POLYA and HEURISTICS

*“[I]ntuition 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.” (George Polya)\**



*\*In *Mathematical Discovery: On Understanding, Learning and Teaching Problem Solving*, 1968.*

## Polya on Picture-writing

$$\begin{aligned}
 & (\square + \textcircled{1} + \textcircled{1}\textcircled{1} + \textcircled{1}\textcircled{1}\textcircled{1} + \dots) \cdot \\
 & (\square + \textcircled{5} + \textcircled{5}\textcircled{5} + \textcircled{5}\textcircled{5}\textcircled{5} + \dots) \cdot \\
 & (\square + \textcircled{10} + \textcircled{10}\textcircled{10} + \textcircled{10}\textcircled{10}\textcircled{10} + \dots) \cdot \\
 & (\square + \textcircled{25} + \textcircled{25}\textcircled{25} + \textcircled{25}\textcircled{25}\textcircled{25} + \dots) \cdot \\
 & (\square + \textcircled{50} + \textcircled{50}\textcircled{50} + \textcircled{50}\textcircled{50}\textcircled{50} + \dots) \cdot \\
 & = \dots + \square \cdot \textcircled{5}\textcircled{5}\textcircled{5} \cdot \textcircled{10} \cdot \textcircled{25} \cdot \textcircled{50} + \dots
 \end{aligned}$$

### Polya's illustration of the change solution

Polya, in his 1956 *American Mathematical Monthly* article provided three provoking examples of converting pictorial representations of problems into generating function solutions. We discuss the first one.

1. *In how many ways can you make change for a dollar?*

This leads to the (US currency) generating function  $\sum_{k \geq 0} P_k x^k =$

$$\frac{1}{(1-x)(1-x^5)(1-x^{10})(1-x^{25})(1-x^{50})}$$

which one can easily expand using a *Mathematica* command,

Series[

```
1/((1-x)*(1-x^5)*(1-x^10)*(1-x^25)*(1-x^50))  
,{x,0,100}]
```

to obtain  $P_{100} = 292$  (**243** for Canadian currency, which lacks a 50 cent piece but has a dollar coin).

- Polya's diagram is shown in the Figure.\*

\*Illustration courtesy the Mathematical Association of America

- To see why, we use geometric series and consider the so called *ordinary generating function*

$$\frac{1}{1 - x^{10}} = 1 + x^{10} + x^{20} + x^{30} + \dots$$

for dimes and

$$\frac{1}{1 - x^{25}} = 1 + x^{25} + x^{50} + x^{75} + \dots$$

for quarters etc.

- We multiply these two together and compare coefficients

$$\begin{aligned} \frac{1}{1 - x^{10}} \frac{1}{1 - x^{25}} &= 1 + x^{10} + x^{20} + x^{25} \\ &+ x^{30} + x^{35} + x^{40} + x^{45} \\ &+ 2x^{50} + x^{55} + 2x^{60} + \dots \end{aligned}$$

We argue that the *coefficient* of  $x^{60}$  on the right is precisely the number of ways of making 60 cents out of identical dimes and quarters.

- This is easy to check with a handful of change or a calculator, The general question with more denominations is handled similarly.
- I leave it open whether it is easier to decode the generating function from the picture or vice versa. In any event, symbolic and graphic experiment provide abundant and mutual reinforcement and assistance in concept formation.

*“In the first place, the beginner must be convinced that proofs deserve to be studied, that they have a purpose, that they are interesting.”* (George Polya)

While by ‘beginner’ George Polya intended young school students, I suggest this is equally true of anyone engaging for the first time with an unfamiliar topic in mathematics.



## MOORE'S LAW

*The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. ... Certainly over the short term this rate can be expected to continue, if not to increase. Over the longer term, the rate of increase is a bit more uncertain, although there is no reason to believe it will not remain nearly constant for at least 10 years.*

(Gordon Moore, Intel co-founder, 1965)

- ▶ “Moore’s Law” asserts that semiconductor technology approximately doubles in capacity and performance roughly every 18 to 24 months (not quite every year as Moore predicted).

This trend has continued unabated for 40 years, and, according to Moore and others, there is still no end in sight—at least another ten years is assured.

► This astounding record of sustained exponential progress has no peer in the history of technology.



What's more, mathematical computing tools are now being implemented on parallel computer platforms, which will provide even greater power to the research mathematician.

► Amassing huge amounts of processing power will not solve all mathematical problems, even those amenable to computational analysis.

There are cases where a dramatic increase in computation could, by itself, result in significant breakthroughs, but it is easier to find examples where this is unlikely to happen.

## **SIMON and RUSSELL**

*This skyhook-skyscraper construction of science from the roof down to the yet unconstructed foundations was possible because the behaviour of the system at each level depended only on a very approximate, simplified, abstracted characterization at the level beneath.<sup>13</sup>*

*This is lucky, else the safety of bridges and airplanes might depend on the correctness of the “Eightfold Way” of looking at elementary particles.*

- ◇ Herbert A. Simon, *The Sciences of the Artificial*, MIT Press, 1996, page 16. (An early experimental computational scientist.)

13... More than fifty years ago Bertrand Russell made the same point about the architecture of mathematics. See the "Preface" to *Principia Mathematica* "... the chief reason in favour of any theory on the principles of mathematics must always be inductive, i.e., it must lie in the fact that the theory in question allows us to deduce ordinary mathematics. In mathematics, the greatest degree of self-evidence is usually not to be found quite at the beginning, but at some later point; hence the early deductions, until they reach this point, give reason rather for believing the premises because true consequences follow from them, than for believing the consequences because they follow from the premises." Contemporary preferences for deductive formalisms frequently blind us to this important fact, which is no less true today than it was in 1910.

## VISUAL DYNAMICS

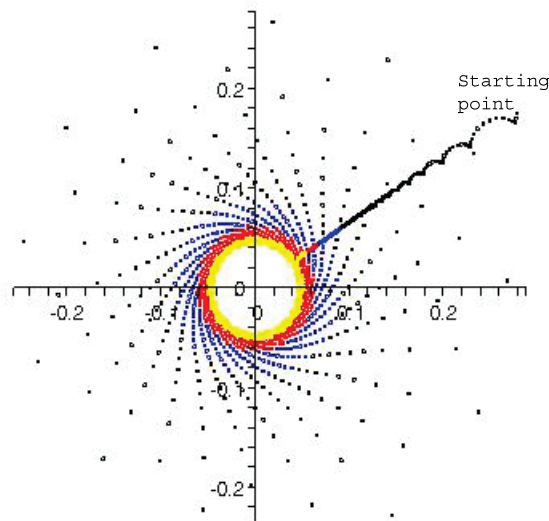
- In recent continued fraction work, we needed to study the *dynamical system*  $t_0 := t_1 := 1$ :

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

where  $\omega_n = a^2, b^2$  for  $n$  even, odd respectively.

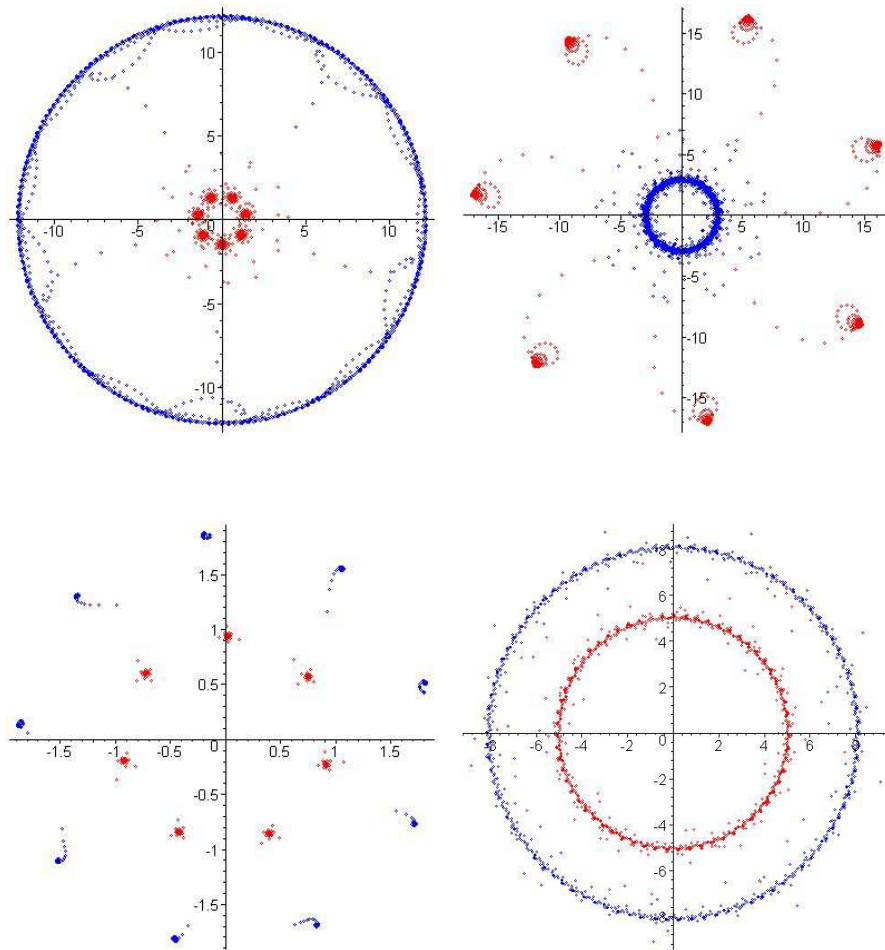
✓ Think of this as a **black box**.

- ▷ Numerically all one sees is  $t_n \rightarrow 0$  slowly.
- ▷ Pictorially we *learn* significantly more\*:



\*... “Then felt I like a watcher of the skies, when a new planet swims into his ken.” (*Chapman’s Homer*)

- Scaling by  $\sqrt{n}$ , and coloring odd and even iterates, fine structure appears.



The **attractors** for various  $|a| = |b| = 1$ .

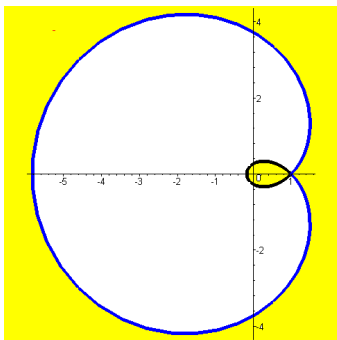
## RAMANUJAN'S FRACTION

Chapter 18 of *Ramanujan's Second Notebook* studies the beautiful:

$$\mathcal{R}_\eta(a, b) = \frac{a}{\eta + \frac{b^2}{\eta + \frac{4a^2}{\eta + \frac{9b^2}{\eta + \dots}}}} \quad (1.1)$$

for **real, positive**  $a, b, \eta > 0$ . Remarkably,  $\mathcal{R}$  satisfies an *AGM relation*

$$\mathcal{R}_\eta\left(\frac{a+b}{2}, \sqrt{ab}\right) = \frac{\mathcal{R}_\eta(a, b) + \mathcal{R}_\eta(b, a)}{2} \quad (1.2)$$



**A scatter plot experiment** discovered the domain of convergence for  $a/b \in \mathbb{C}$ . This is now fully explained with a *lot* of dynamics work.

## GAUSS and HADAMARD

Carl Friedrich Gauss, who drew (carefully) and computed a great deal, once noted, *I have the result, but I do not yet know how to get it.*\*



**Pauca sed Matura**

*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.

\*Likewise the quote!



Sic lenitate, elegantissime omnes expectationes  
 superantia acquisitionibus et quibus  
 per methodos quae campum profusus  
 nunc nobis aperunt. Gott. Jul.

# Solutio problematis ballistici Gott. Jul.

# Comentarum theoriam perfectiorum reddidi Gott. Jul.

Novus in analysi campus se nobis aperuit  
 scilicet investigatio functionum etc.

# Formas superiores considerare coepimus  
 Formulas novas exactas pro parallaxi  
 erimus ————— Mr. Apr. 8.

# Terminum medium arithmetico-geometricum  
 inter 1 et  $\sqrt{2}$  esse =  $\frac{\pi}{10}$  vique  
 ad huc usque invidiam comprobavimus, quare  
 demonstrata proinde novus campus in analysi  
 certo aperitur Mr. Mai 30.

# In principis Geometriae egregios progressus  
 fecimus Mr. Sept. 1798

# Circa terminos medios arithmetico-geometricos  
 multi nova detegimus. Mr. Novemb.

## Novus in analysi campus se nobis aperuit

An excited young Gauss writes: “A new field of analysis has appeared to us, evidently in the study of functions etc.” (October 1798)

## MOTIVATION and GOALS

**INSIGHT** – demands speed  $\equiv$  **micro-parallelism**

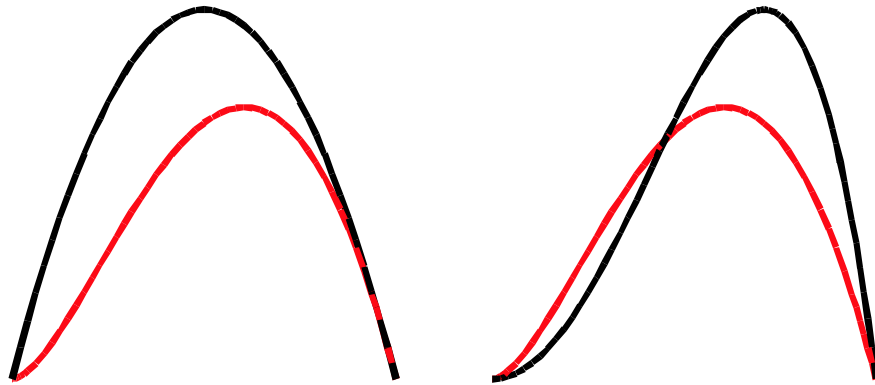
- For rapid verification.
- For validation; proofs *and* refutations; “monster barring”.
- ★ What is “easy” changes: HPC & HPN blur, merging disciplines and collaborators — democratizing mathematics but challenging authenticity.
- **Parallelism**  $\equiv$  more space, speed & stuff.
- **Exact**  $\equiv$  hybrid  $\equiv$  symbolic ‘+’ numeric (*Maple meets NAG*).
- In analysis, algebra, geometry & topology.

## ... MOREOVER

- Towards an Experimental **Methodology** — philosophy and practice.
- ▶ **Intuition is acquired** — mesh computation and mathematics.
- **Visualization** — **3** is a lot of dimensions.
- ▶ “Monster-barring” (Lakatos) and “Caging”:
  - randomized checks: equations, linear algebra, primality.
  - graphic checks: equalities, inequalities, areas.

## Graphic Checks

- Comparing  $y - y^2$  and  $y^2 - y^4$  to  $-y^2 \ln(y)$  for  $0 < y < 1$  pictorially is a much more rapid way to divine which is larger than traditional analytic methods.
- It is clear that in the later case they cross, it is futile to try to prove one majorizes the other. In the first case, evidence is provided to motivate a proof.



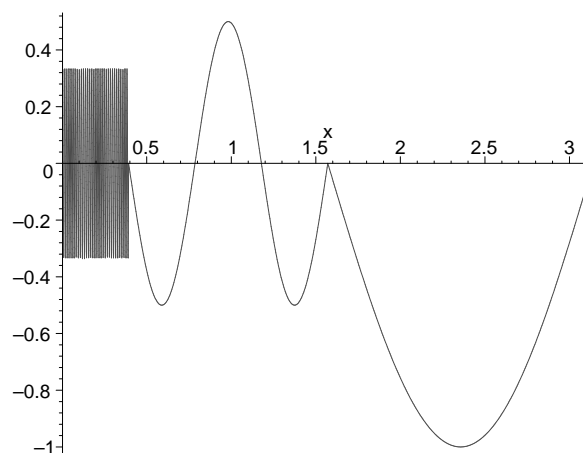
**Graphical comparison of**  
 $y - y^2$  and  $y^2 - y^4$  to  $-y^2 \ln(y)$  (red)

## EXPERIMENTAL MATHODOLOGY.

1. Gaining insight and intuition.
2. Discovering new patterns and relationships.
3. Graphing to expose 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.

## A BRIEF HISTORY OF RIGOUR

- Greeks: trisection, circle squaring, cube doubling and  $\sqrt{2}$ .
- Newton and Leibniz: fluxions and infinitesimals.
- Cauchy and Fourier: limits and continuity.
- Frege and Russell, Gödel and Turing.



**Fourier series need not converge**

## THE PHILOSOPHIES OF RIGOUR

- Everyman: **Platonism**—stuff exists (1936)
- Hilbert: **Formalism**—math is invented; formal symbolic games without meaning
- Brouwer: **Intuitionism**—many variants; (embodied cognition)
- Bishop: **Constructivism**—tell me how big; (social constructivism)

† Last two deny the *excluded middle*:  $A \vee \tilde{A}$

## HALES and KEPLER

- Kepler's conjecture: **the densest way to stack spheres is in a pyramid** is the oldest problem in discrete geometry.
- The most interesting recent example of computer assisted proof. Published in *Annals of Math* with an "only 99% checked" disclaimer.
- This has triggered very varied reactions. (In Math, Computers Don't Lie. Or Do They? *NYT* 6/4/04)
- Famous earlier examples: **The Four Color Theorem** and **The non existence of a projective plane of order 10.**
- The three raise and answer quite distinct questions—both real and specious.



## Does the proof stack up?

Think peer review takes too long? One mathematician has waited four years to have his paper refereed, only to hear that the exhausted reviewers can't be certain whether his proof is correct. George Szpiro investigates.

P. TURNLEYS, SHERRELL/R. BICKEL/CORBIS, H. SITTON/GETTY



Grocers the world over know the most efficient way to stack spheres — but a mathematical proof for the method has brought reviewers to their knees.

Just under five years ago, Thomas Hales made a startling claim. In an e-mail he sent to dozens of mathematicians, Hales declared that he had used a series of computers to prove an idea that has evaded certain confirmation for 400 years. The subject of his message was Kepler's conjecture, proposed by the German astronomer Johannes Kepler, which states that the densest arrangement of spheres is one in which they are stacked in a pyramid — much the same way as grocers arrange oranges.

Soon after Hales made his announcement, reports of the breakthrough appeared on the front pages of newspapers around the world. But today, Hales's proof remains in limbo. It has been submitted to the prestigious *Annals of Mathematics*, but is yet to appear in print. Those charged with checking it say that they believe the proof is correct, but are so exhausted with the verification process that they cannot definitively rule out any errors. So when Hales's manuscript finally does appear in the *Annals*, probably during the next year, it will carry an unusual editorial note — a statement that parts of the paper have proved impossible to check.

At the heart of this bizarre tale is the use of computers in mathematics, an issue that has split the field. Sometimes described as a 'brute force' approach, computer-aided

proofs often involve calculating thousands of possible outcomes to a problem in order to produce the final solution. Many mathematicians dislike this method, arguing that it is inelegant. Others criticize it for not offering any insight into the problem under consideration. In 1977, for example, a computer-aided proof was published for the four-colour theorem, which states that no more than four colours are needed to fill in a map so that any two adjacent regions have different colours<sup>1,2</sup>. No errors have been found in the proof, but some mathematicians continue to seek a solution using conventional methods.

### Pile-driver

Hales, who started his proof at the University of Michigan in Ann Arbor before moving to the University of Pittsburgh, Pennsylvania, began by reducing the infinite number of possible stacking arrangements to 5,000 contenders. He then used computers to calculate the density of each arrangement. Doing so was more difficult than it sounds. The proof involved checking a series of mathematical inequalities using specially written computer code. In all, more than 100,000 inequalities were verified over a ten-year period.

Robert MacPherson, a mathematician at the Institute for Advanced Study in Princeton, New Jersey, and an editor of the *Annals*,

was intrigued when he heard about the proof. He wanted to ask Hales and his graduate student Sam Ferguson, who had assisted with the proof, to submit their finding for publication, but he was also uneasy about the computer-based nature of the work.

The *Annals* had, however, already accepted a shorter computer-aided proof — the paper, on a problem in topology, was published this March<sup>3</sup>. After sounding out his colleagues on the journal's editorial board, MacPherson asked Hales to submit his paper. Unusually, MacPherson assigned a dozen mathematicians to referee the proof — most journals tend to employ between one and three. The effort was led by Gábor Fejes Tóth of the Alfréd Rényi Institute of Mathematics in Budapest, Hungary, whose father, the mathematician László Fejes Tóth, had predicted in 1965 that computers would one day make a proof of Kepler's conjecture possible.

It was not enough for the referees to rerun Hales's code — they had to check whether the programs did the job that they were supposed to do. Inspecting all of the code and its inputs and outputs, which together take up three gigabytes of memory space, would have been impossible. So the referees limited themselves to consistency checks, a reconstruction of the thought processes behind each step of the proof, and then a

S. TERRY/SPL

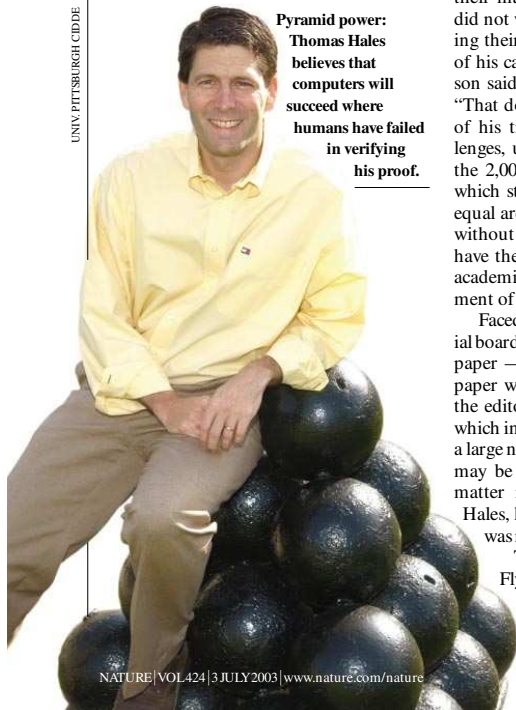
study of all of the assumptions and logic used to design the code. A series of seminars, which ran for full academic years, was organized to aid the effort.

But success remained elusive. Last July, Fejes Tóth reported that he and the other referees were 99% certain that the proof is sound. They found no errors or omissions, but felt that without checking every line of the code, they could not be absolutely certain that the proof is correct.

For a mathematical proof, this was not enough. After all, most mathematicians believe in the conjecture already—the proof is supposed to turn that belief into certainty. The history of Kepler's conjecture also gives reason for caution. In 1993, Wu-Yi Hsiang, then at the University of California, Berkeley, published a 100-page proof of the conjecture in the *International Journal of Mathematics*<sup>4</sup>. But shortly after publication, errors were found in parts of the proof. Although Hsiang stands by his paper, most mathematicians do not believe it is valid.

After the referees' reports had been considered, Hales says that he received the following letter from MacPherson: "The news from the referees is bad, from my perspective. They have not been able to certify the correctness of the proof, and will not be able to certify it in the future, because they have run out of energy... One can speculate whether their process would have converged to a definitive answer had they had a more clear manuscript from the beginning, but this does not matter now."

UNIV. PITTSBURGH CIDDE



**Pyramid power:**  
Thomas Hales believes that computers will succeed where humans have failed in verifying his proof.

NATURE | VOL 424 | 3 JULY 2003 | www.nature.com/nature



**Star player:** Johannes Kepler's conjecture has kept mathematicians guessing for 400 years.

The last sentence lets some irritation shine through. The proof that Hales delivered was by no means a polished piece. The 250-page manuscript consisted of five separate papers, each a sort of lab report that Hales and Ferguson filled out whenever the computer finished part of the proof. This unusual format made for difficult reading. To make matters worse, the notation and definitions also varied slightly between the papers.

#### Rough but ready

MacPherson had asked the authors to edit their manuscript. But Hales and Ferguson did not want to spend another year reworking their paper. "Tom could spend the rest of his career simplifying the proof," Ferguson said when they completed their paper. "That doesn't seem like an appropriate use of his time." Hales turned to other challenges, using traditional methods to solve the 2,000-year-old honeycomb conjecture, which states that of all conceivable tiles of equal area that can be used to cover a floor without leaving any gaps, hexagonal tiles have the shortest perimeter<sup>5</sup>. Ferguson left academia to take a job with the US Department of Defense.

Faced with exhausted referees, the editorial board of the *Annals* decided to publish the paper — but with a cautionary note. The paper will appear with an introduction by the editors stating that proofs of this type, which involve the use of computers to check a large number of mathematical statements, may be impossible to review in full. The matter might have ended there, but for Hales, having a note attached to his proof was not satisfactory.

This January, he launched the Flyspeck project, also known as the Formal Proof of Kepler. Rather than rely on human referees, Hales intends to use computers to verify

every step of his proof. The effort will require the collaboration of a core group of about ten volunteers, who will need to be qualified mathematicians and willing to donate the computer time on their machines. The team will write programs to deconstruct each step of the proof, line by line, into a set of axioms that are known to be correct. If every part of the code can be broken down into these axioms, the proof will finally be verified.

Those involved see the project as doing more than just validating Hales's proof. Sean McLaughlin, a graduate student at New York University, who studied under Hales and has used computer methods to solve other mathematical problems, has already volunteered. "It seems that checking computer-assisted proofs is almost impossible for humans," he says. "With luck, we will be able to show that problems of this size can be subjected to rigorous verification without the need for a referee process."

But not everyone shares McLaughlin's enthusiasm. Pierre Deligne, an algebraic geometer at the Institute for Advanced Study, is one of the many mathematicians who do not approve of computer-aided proofs. "I believe in a proof if I understand it," he says. For those who side with Deligne, using computers to remove human reviewers from the refereeing process is another step in the wrong direction.

Despite his reservations about the proof, MacPherson does not believe that mathematicians should cut themselves off from computers. Others go further. Freek Wiedijk, of the Catholic University of Nijmegen in the Netherlands, is a pioneer of the use of computers to verify proofs. He thinks that the process could become standard practice in mathematics. "People will look back at the turn of the twentieth century and say that is when it happened," Wiedijk says.

Whether or not computer-checking takes off, it is likely to be several years before Flyspeck produces a result. Hales and McLaughlin are the only confirmed participants, although others have expressed an interest. Hales estimates that the whole process, from crafting the code to running it, is likely to take 20 person-years of work. Only then will Kepler's conjecture become Kepler's theorem, and we will know for sure whether we have been stacking oranges correctly all these years. ■

George Szpiro writes for the Swiss newspapers *NZZ* and *NZZ am Sonntag* from Jerusalem, Israel. His book *Kepler's Conjecture* (Wiley, New York) was published in February.

1. Appel, K. & Haken, W. *Illinois J. Math.* **21**, 429–490 (1977).
2. Appel, K., Haken, W. & Koch, J. *Illinois J. Math.* **21**, 491–567 (1977).
3. Gabai, D., Meyerhoff, G. R. & Thurston, N. *Ann. Math.* **157**, 335–431 (2003).
4. Hsiang, W.-Y. *Int. J. Math.* **4**, 739–831 (1993).
5. Hales, T. C. *Discrete Comput. Geom.* **25**, 1–22 (2001).

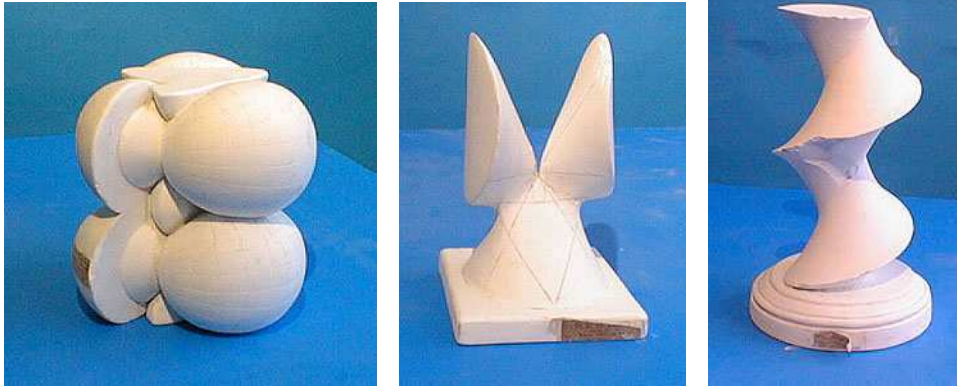
Flyspeck

► [www.math.pitt.edu/~thales/flyspeck/index.html](http://www.math.pitt.edu/~thales/flyspeck/index.html)

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## 19th C. MATHEMATICAL MODELS



### Felix Klein's heritage

*Considerable obstacles generally present themselves to the beginner, in studying the elements of Solid Geometry, from the practice which has hitherto uniformly prevailed in this country, of never submitting to the eye of the student, the figures on whose properties he is reasoning, but of drawing perspective representations of them upon a plane. ...*

*I hope that I shall never be obliged to have recourse to a perspective drawing of any figure whose parts are not in the same plane.*

Augustus de Morgan (1806–71).

- de Morgan, first President of the London Mathematical Society, was equally influential as an educator and a researcher.
- There is evidence that young children see more naturally in three than two dimensions.

(See discussion at [www.colab.sfu.ca/ICIAM03/](http://www.colab.sfu.ca/ICIAM03/))



**Coxeter's octahedral kaleidoscope  
(circa 1925)**

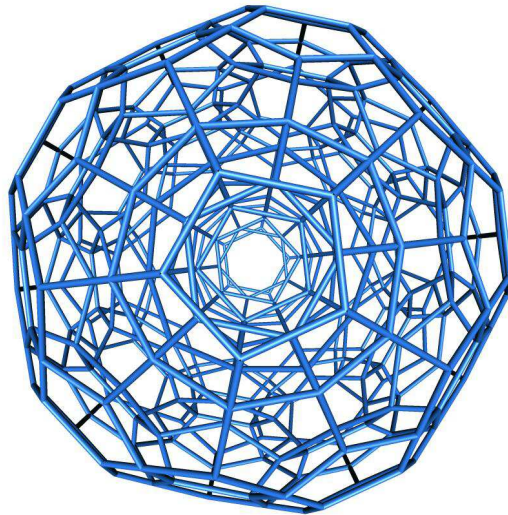
*Modern science is often driven by fads and fashion, and mathematics is no exception. Coxeter's style, I would say, is singularly unfashionable. He is guided, I think, almost completely by a profound sense of what is beautiful.*

(Robert Moody)

*Mathematics, rightly viewed, possesses not only truth, but supreme beauty—a beauty cold and austere, without appeal to any part of our weaker nature, without the gorgeous trappings of painting or music, yet sublimely pure, and capable of a stern perfection such as only the greatest art can show.*

(Bertrand Russell, 1910)

- Quoted in the introduction to Coxeter's *Introduction to Geometry*.
- Russell, a family friend, may have been responsible for Coxeter pursuing mathematics. After reading the 16 year old's prize-winning essay on *dimensionality*, he told Coxeter's father his son was unusually gifted mathematically, and urged him to change the direction of Coxeter's education.



## **A four dimensional polytope with 120 dodecahedral faces**

- In a **1997** paper, Coxeter showed his friend Escher, knowing no math, had achieved “mathematical perfection” in etching *Circle Limit III*. “Escher did it by instinct,” Coxeter wrote, “I did it by trigonometry.”
- Fields medalist David Mumford recently noted that Donald Coxeter (**1907-2003**) placed great value on working out details of complicated explicit examples.

*In my book, Coxeter has been one of the most important 20th century mathematicians —not because he started a new perspective, but because he deepened and extended so beautifully an older esthetic. The classical goal of geometry is the exploration and enumeration of geometric configurations of all kinds, their symmetries and the constructions relating them to each other.*

*The goal is not especially to prove theorems but to discover these perfect objects and, in doing this, theorems are only a tool that imperfect humans need to reassure themselves that they have seen them correctly.*

(David Mumford, 2003)

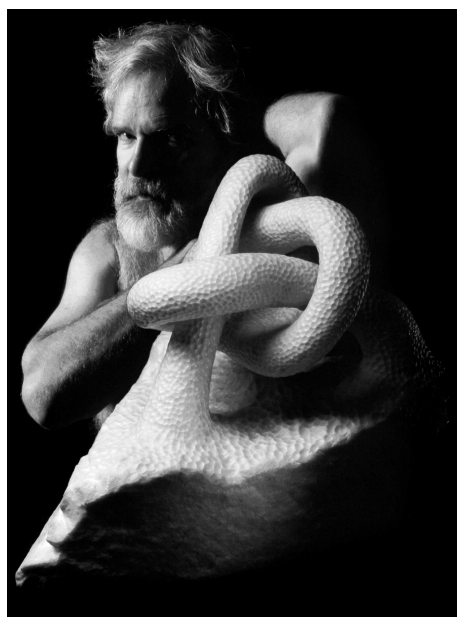


## 20th C. MATHEMATICAL MODELS



Ferguson's "Eight-Fold Way" sculpture

The Fergusons won the 2002 Communications Award, of the Joint Policy Board of Mathematics. The citation runs:



*They have dazzled the mathematical community and a far wider public with exquisite sculptures embodying mathematical ideas, along with artful and accessible essays and lectures elucidating the mathematical concepts.*

It has been known for some time that the *hyperbolic volume*  $V$  of the **figure-eight knot complement** is

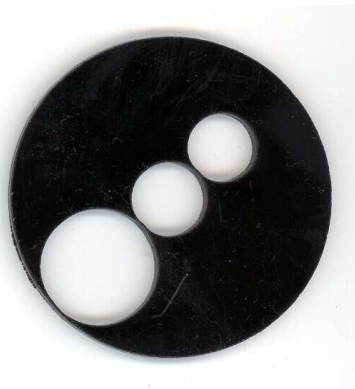
$$\begin{aligned}
 V &= 2\sqrt{3} \sum_{n=1}^{\infty} \frac{1}{n \binom{2n}{n}} \sum_{k=n}^{2n-1} \frac{1}{k} \\
 &= 2.029883212819307250042405108549 \dots
 \end{aligned}$$



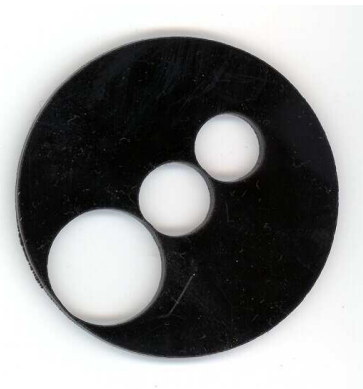
**Ferguson's "Figure-Eight Knot Complement" sculpture**

In 1998, British physicist David Broadhurst conjectured  $V/\sqrt{3}$  is a *rational linear combination* of

$$(2) \quad C_j = \sum_{n=0}^{\infty} \frac{(-1)^n}{27^n (6n + j)^2}.$$



Ferguson's  
subtractive  
image  
of the  
**BBP Pi**  
formula



Indeed, as Broadhurst found, *using Ferguson's PSLQ*:

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

- Entering the following code in the *Mathematician's Toolkit*, at [www.expmath.info](http://www.expmath.info):

```
v = 2 * sqrt[3] * sum[1/(n * binomial[2*n,n])
    * sum[1/k,{k, n,2*n-1}], {n, 1, infinity}]

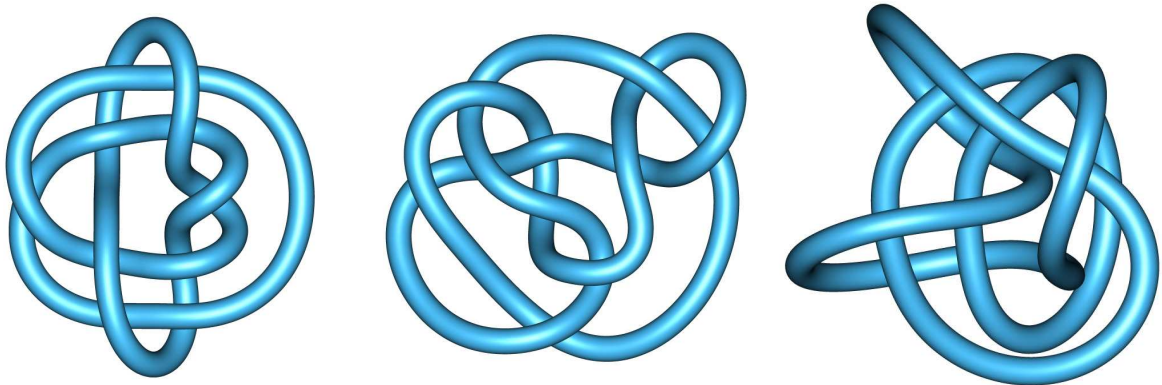
ps1q[v/sqrt[3],
    table[sum[(-1)^n/(27^n*(6*n+j)^2),
{n, 0, infinity}], {j, 1, 6}]]
```

recovers the solution vector

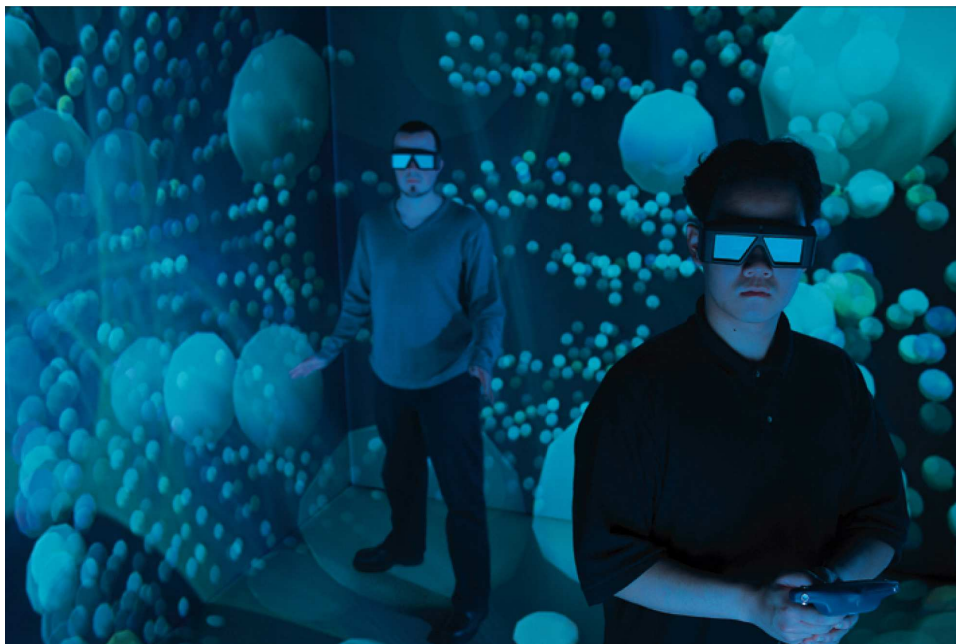
**(9, -18, 18, 24, 6, -2, 0).**

- The *first proof* that this formula holds is given in our new book.
- The formula is inscribed on each cast of the sculpture—marrying both sides of Helaman!

## 21st C. MATHEMATICAL MODELS



Knots  $10_{161}$  (L) and  $10_{162}$  (C) agree (R)\*.



**In NewMIC's Cave or Plato's?**

\***KnotPlot**: from Little (1899) to Perko (1974) and on.

## MORE of OUR 'METHODOLOGY'

1. (*High Precision*) computation of object(s).

2. *Pattern Recognition of Real Numbers*

$$\text{identify}(\sqrt{2} + \sqrt{3}) = \sqrt{2} + \sqrt{3}$$

(Inverse Calculator and 'identify')\* or Sequences (Salvy & Zimmermann's 'gfun', Sloane and Plouffe's *Encyclopedia*).

3. Much use of 'Integer Relation Methods': †

✓ "Exclusion bounds" are especially useful.

✓ Great test bed for "Experimental Math".

4. Some automated theorem proving (Wilf-Zeilberger etc).

\*ISC space limits: from 10Mb in 1985 to 10Gb today.

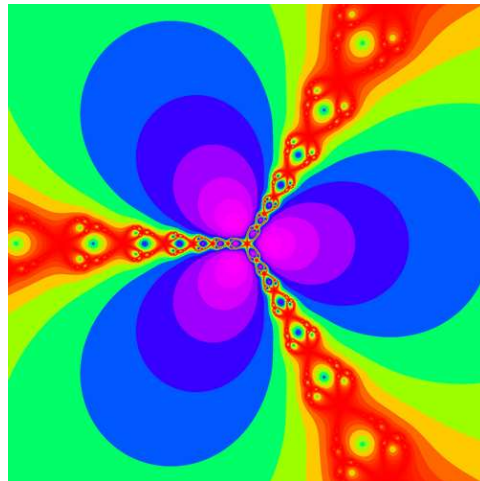
†PSLQ, LLL, FFT. Top Ten "Algorithm's for the Ages," Random Samples, Science, Feb. 4, 2000.

## **FOUR EXPERIMENTS**

- 1. **Kantian** example: generating “the classical non-Euclidean geometries (hyperbolic, elliptic) by replacing Euclid’s axiom of parallels (or something equivalent to it) with alternative forms.”
- 2. The **Baconian** experiment is a contrived as opposed to a natural happening, it “is the consequence of ‘trying things out’ or even of merely messing about.”
- 3. **Aristotelian** demonstrations: “apply electrodes to a frog’s sciatic nerve, and lo, the leg kicks; always precede the presentation of the dog’s dinner with the ringing of a bell, and lo, the bell alone will soon make the dog dribble.”



- 4. The most important is **Galilean**: “a critical experiment – one that discriminates between possibilities and, in doing so, either gives us confidence in the view we are taking or makes us think it in need of correction.”
- It is also the only one of the four forms which will make Experimental Mathematics a serious enterprise.
- From Peter Medawar's *Advice to a Young Scientist*, Harper (1979).

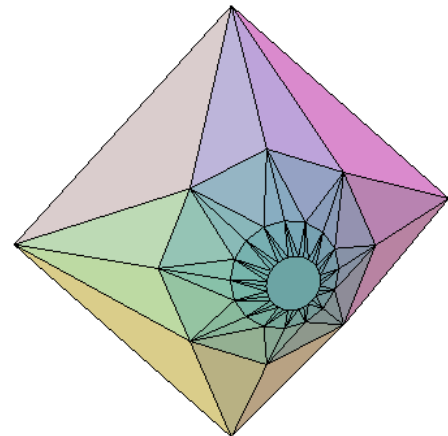


**A Julia set**

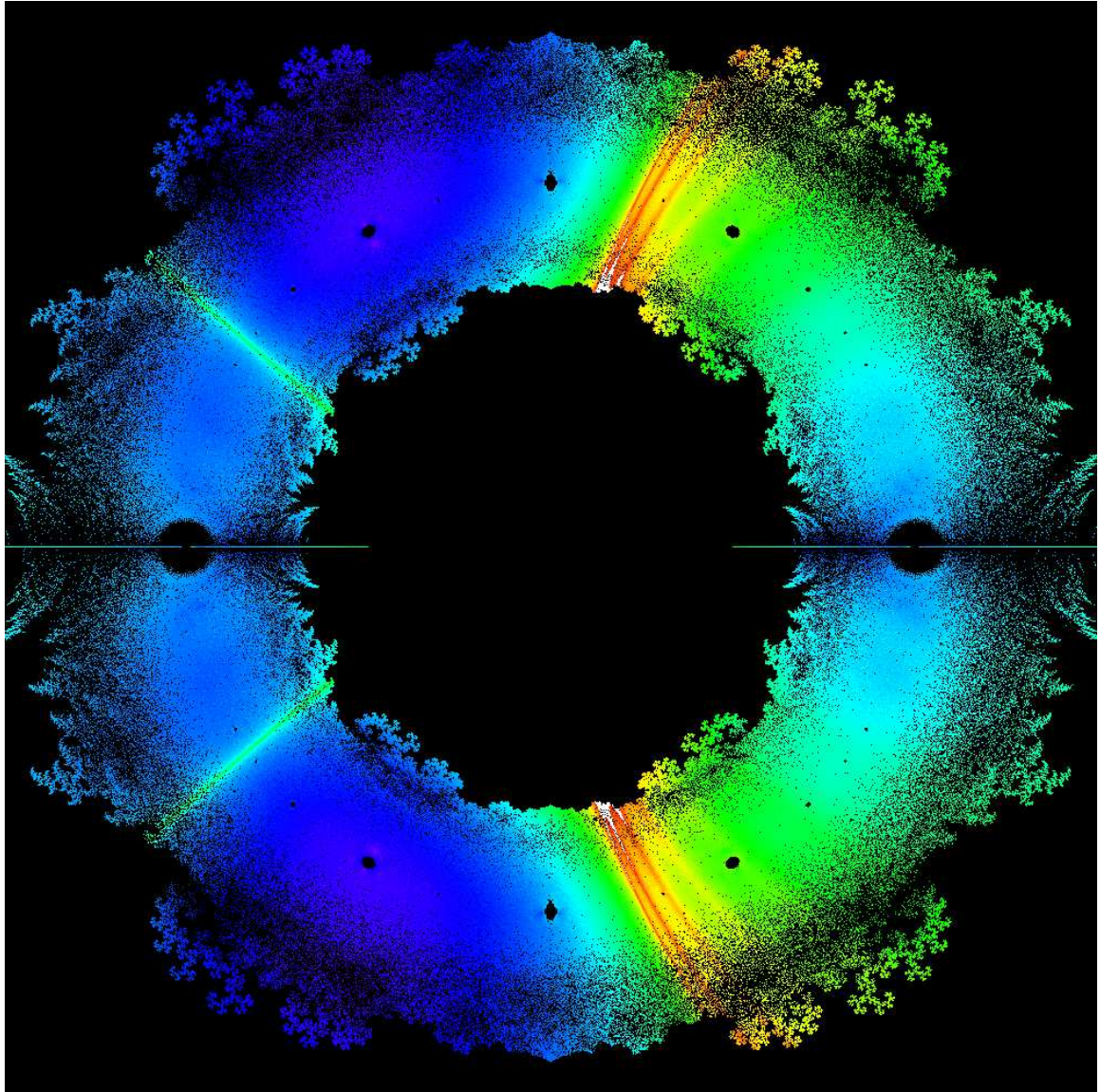
## MILNOR

*If I can give an abstract proof of something, I'm reasonably happy. But if I can get a concrete, computational proof and actually produce numbers I'm much happier.*

*I'm rather an addict of doing things on the computer, because that gives you an explicit criterion of what's going on. I have a visual way of thinking, and I'm happy if I can see a picture of what I'm working with.*



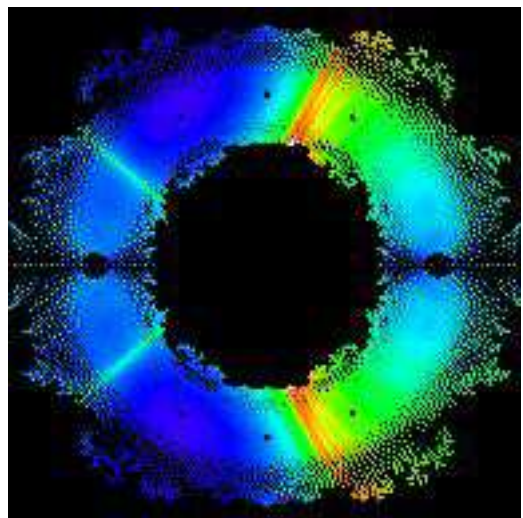
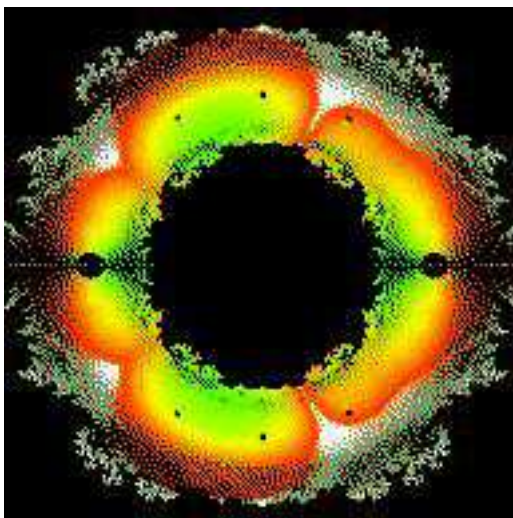
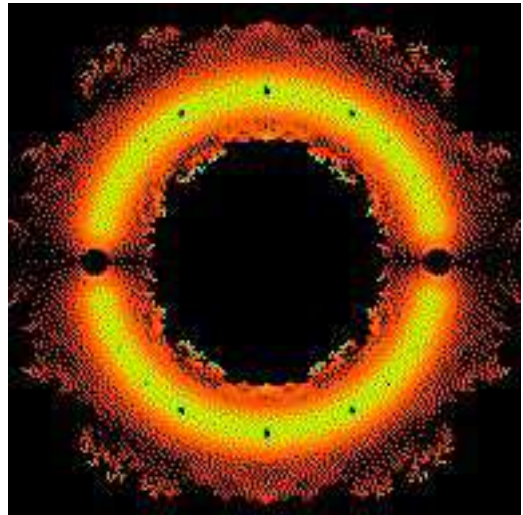
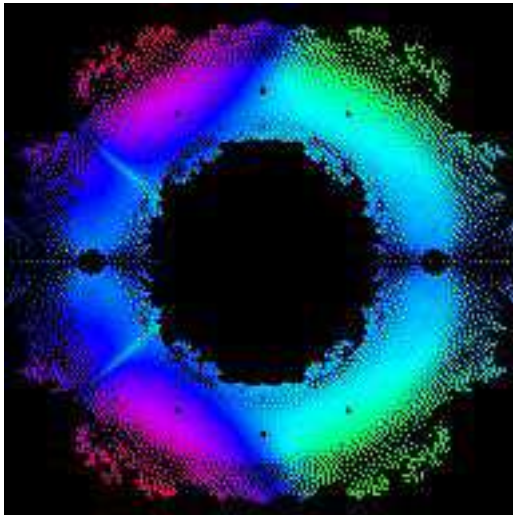
# ZEROES of 0 – 1 POLYNOMIALS



## Data mining in polynomials

- The striations are unexplained!

**WHAT YOU DRAW is WHAT YOU SEE**

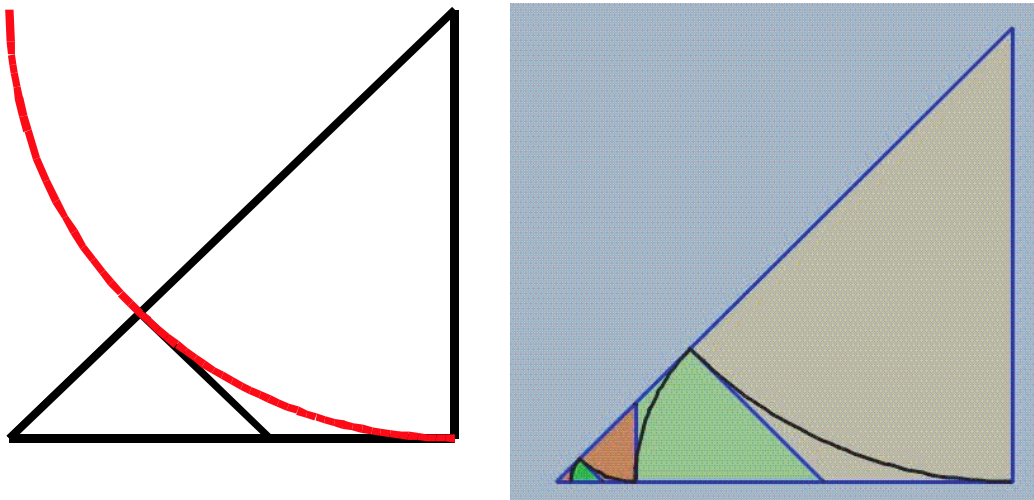


**The price of metaphor is eternal  
vigilance** (Arturo Rosenblueth & Norbert Wiener)

## A NEW PROOF $\sqrt{2}$ is IRRATIONAL

One can find new insights in the oldest areas:

- Here is Tom Apostol's lovely new graphical proof\* of the irrationality of  $\sqrt{2}$ . I like very much that this was published in the present millennium.



**Root two is irrational (static and self-similar pictures)**

\**MAA Monthly*, November 2000, 241–242.

**PROOF.** To say  $\sqrt{2}$  is rational is to draw a right-angled isosceles triangle with integer sides. Consider the *smallest* right-angled isosceles triangle with integer sides —that is with shortest hypotenuse.

Circumscribe a circle of radius the vertical side and construct the tangent on the hypotenuse, as in the picture.

**Repeating the process once more produces an even smaller such triangle in the same orientation as the initial one.**

The *smaller* right-angled isosceles triangle again has integer sides ... . **QED**

**Rationality**  $\sqrt{2}$  also makes things rational:

$$\left(\sqrt{2}\sqrt{2}\right)^{\sqrt{2}} = \sqrt{2}(\sqrt{2}\cdot\sqrt{2}) = \sqrt{2}^2 = 2.$$

Hence by *the principle of the excluded middle*:

$$\text{Either } \sqrt{2}\sqrt{2} \in \mathbb{Q} \text{ or } \sqrt{2}\sqrt{2} \notin \mathbb{Q}.$$

In *either* case we can deduce that there are irrational numbers  $\alpha$  and  $\beta$  with  $\alpha^\beta$  rational. *But how do we know which ones?* Compare the assertion that

$$\alpha := \sqrt{2} \text{ and } \beta := 2 \ln_2(3) \text{ yield } \alpha^\beta = 3$$

as *Mathematica* confirms.

- Again, verification is easier than discovery. Similarly multiplication is easier than factorization, as in secure encryption schemes for e-commerce.

There are eight possible (ir)rational triples:

$$\alpha^\beta = \gamma.$$

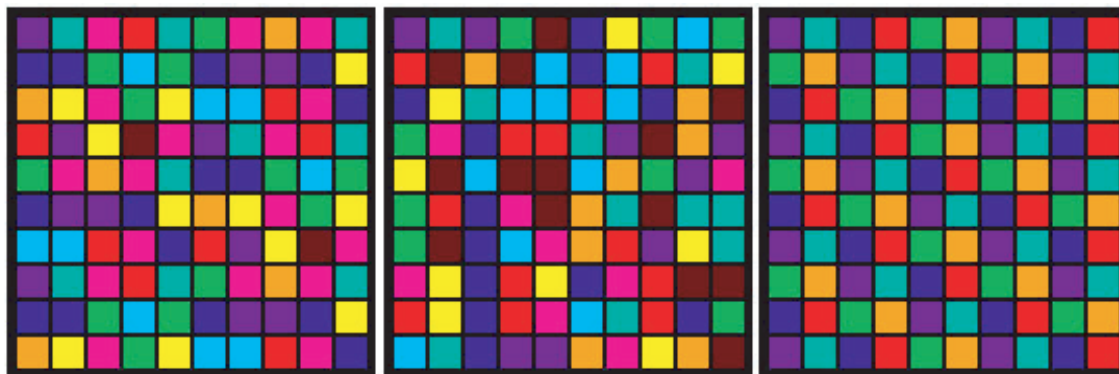
Can you find them?

## TWO INTEGRALS

A. Why  $\pi \neq \frac{22}{7}$ :

$$0 < \int_0^1 \frac{(1-x)^4 x^4}{1+x^2} dx = \frac{22}{7} - \pi.$$

$$\left[ \int_0^t \cdot = \frac{1}{7}t^7 - \frac{2}{3}t^6 + t^5 - \frac{4}{3}t^3 + 4t - 4 \arctan(t) \right]$$



Archimedes:  $\frac{223}{71} < \pi < \frac{22}{7}$

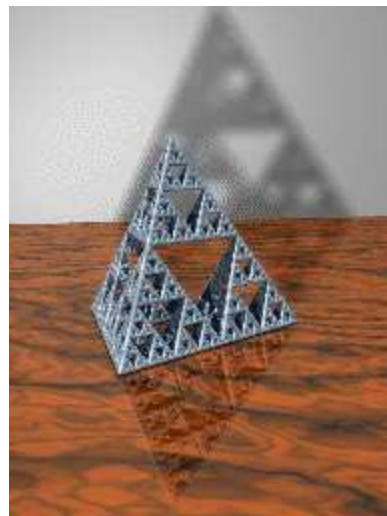
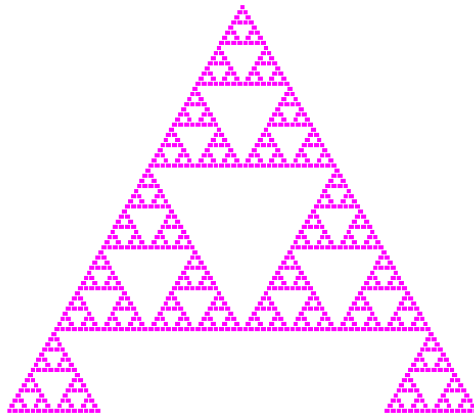
The Colour Calculator



**B.** *The sophomore's dream* (Found by John Bernoulli, 1697.):

$$\int_0^1 \frac{1}{x^x} dx = \sum_{n=1}^{\infty} \frac{1}{n^n}.$$

- Such have many implications for teaching — flagging issues of ‘Packing and unpacking’ concepts?



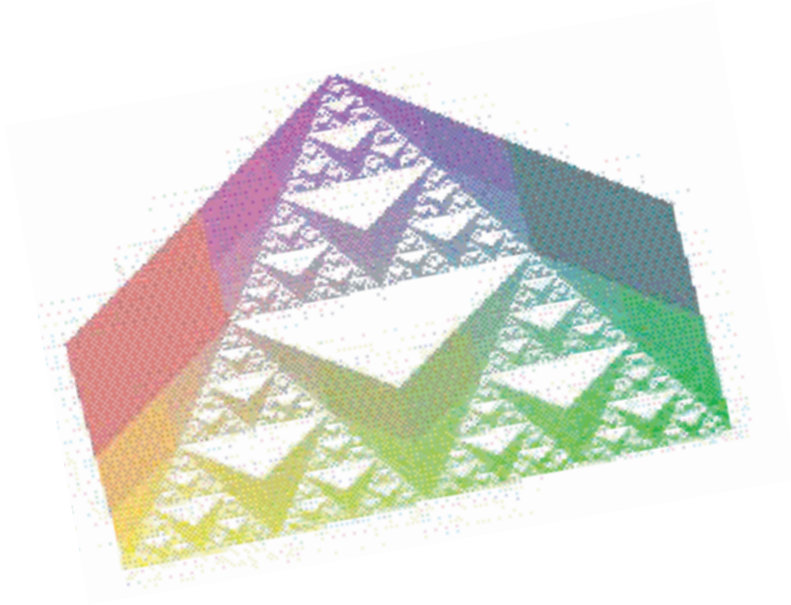
**Pascal's Triangle modulo two**

**1**, 1 1, **1 2 1**, 1 3 3 1, **1 4 6 4 1**, 1 5 10 10 5 1 ...

## FRACTAL CARDS

Not all impressive discoveries require a computer.

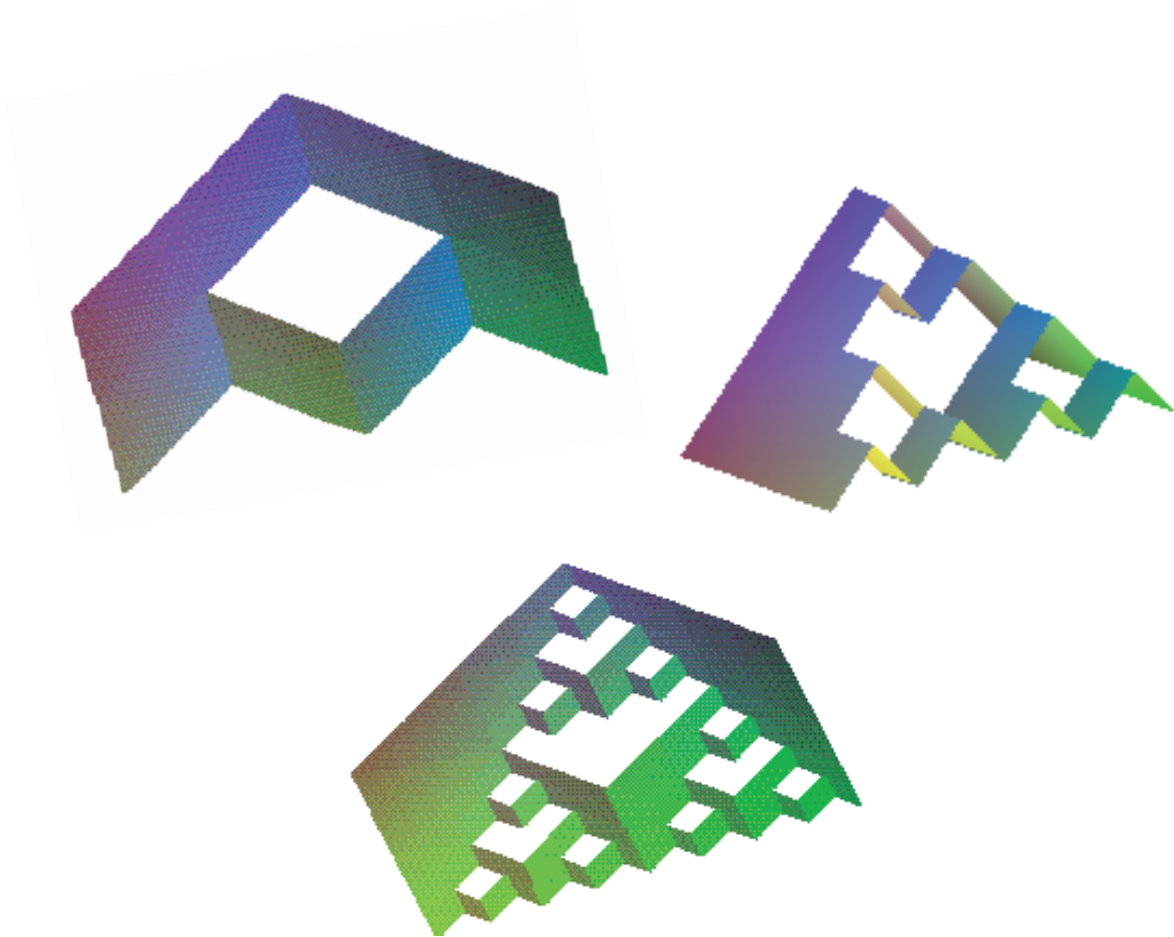
Elaine Simmt and Brent Davis describe lovely constructions made by repeated regular paper folding and cutting—but no removal of paper—that result in beautiful fractal, self-similar, “pop-up” cards\*.



### The 7th iterates of a Sierpinski triangle

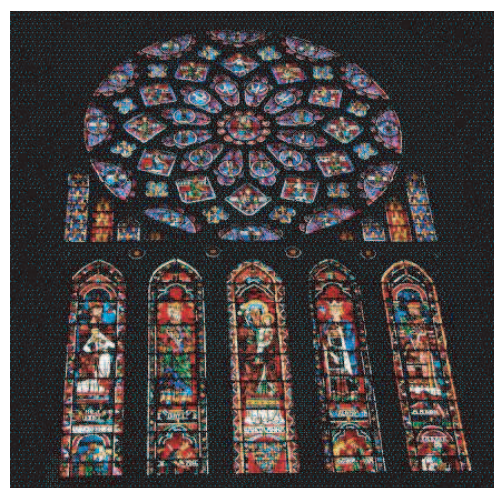
\*Fractal Cards: A Space for Exploration in Geometry and Discrete Maths, *Math Teacher*, **91** (1998), 102-8

- Nonetheless, we show various iterates of a pop-up Sierpinski triangle built in software, on turning those paper cutting and folding rules into an algorithm.
- This should let you start folding.



**The 1st, 2nd and 3rd iterates**

- Note the similarity to the **Pascal triangle**.
- And always art can be an additional source of mathematical inspiration and stimulation



## Self similarity at Chartres

## TWO INFINITE PRODUCTS

A. A rational evaluation:

$$\prod_{n=2}^{\infty} \frac{n^3 - 1}{n^3 + 1} = \frac{2}{3}.$$

...

B. And a transcendent one:

$$\prod_{n=2}^{\infty} \frac{n^2 - 1}{n^2 + 1} = \frac{\pi}{\sinh(\pi)}.$$

- The *Inverse Symbolic Calculator* can identify this product, as can **Maple**.
- $\int, \Sigma, \Pi$  are now largely algorithmic not **black arts**.

## COINCIDENCE OR FRAUD

- Coincidences do occur

The approximations

$$\pi \approx \frac{3}{\sqrt{163}} \log(640320)$$

and

$$\pi \approx \sqrt{2} \frac{9801}{4412}$$

occur for deep number theoretic reasons—the first good to 15 places, the second to eight. By contrast

$$e^\pi - \pi = \mathbf{19.999099979}189475768\dots$$

most probably for no good reason.

- ✓ This seemed more bizarre on an eight digit calculator.

Likewise, as spotted by Pierre Lanchon recently,

$$e = \overline{\mathbf{10.10110111111000010}}101000101100\dots$$

while

$$\pi = 11.0010\overline{\mathbf{010000111110110101}}01000\dots$$

have 19 bits agreeing in base two—with one read right to left.

- More extended coincidences are almost always contrived ...

## HIGH PRECISION FRAUD

$$\sum_{n=1}^{\infty} \frac{[n \tanh(\pi)]}{10^n} \stackrel{?}{=} \frac{1}{81}$$

is valid to **268 places**; while

$$\sum_{n=1}^{\infty} \frac{[n \tanh(\frac{\pi}{2})]}{10^n} \stackrel{?}{=} \frac{1}{81}$$

is valid to just **12 places**.

- Both are actually transcendental numbers.

Correspondingly the *simple continued fractions* for  $\tanh(\pi)$  and  $\tanh(\frac{\pi}{2})$  are respectively

[0, 1, **267**, 4, 14, 1, 2, 1, 2, 2, 1, 2, 3, 8, 3, 1]

and

[0, 1, **11**, 14, 4, 1, 1, 1, 3, 1, 295, 4, 4, 1, 5, 17, 7]

- Bill Gosper describes how continued fractions let you “see” what a number is. “[I]t’s completely astounding ... **it looks like you are cheating God somehow.**”



## SEEING PATTERNS in PARTITIONS

The number of *additive partitions* of  $n$ ,  $p(n)$ , is *generated* by

$$(3) \quad 1 + \sum_{n \geq 1} p(n)q^n = \frac{1}{\prod_{n \geq 1} (1 - q^n)}.$$

Thus,  $p(5) = 7$  since

$$\begin{aligned} 5 &= 4 + 1 = 3 + 2 = 3 + 1 + 1 = 2 + 2 + 1 \\ &= 2 + 1 + 1 + 1 = 1 + 1 + 1 + 1 + 1. \end{aligned}$$

Developing (3) is an introduction to enumeration via *generating functions* as discussed in Polya's change example.

Additive partitions are harder to handle than multiplicative factorizations, but they may be introduced in the elementary school curriculum with questions like: *How many 'trains' of a given length can be built with Cuisenaire rods?*

Ramanujan used MacMahon's table of  $p(n)$  to intuit remarkable deep congruences like

$$p(5n+4) \equiv 0 \pmod{5}, \quad p(7n+5) \equiv 0 \pmod{7}$$

$$p(11n+6) \equiv 0 \pmod{11},$$

from relatively limited data like  $P(q) =$

$$\begin{aligned} &1 + q + 2q^2 + 3q^3 + \underline{5}q^4 + \overline{7}q^5 + 11q^6 + 15q^7 \\ &+ 22q^8 + \underline{30}q^9 + 42q^{10} + 56q^{11} + \overline{77}q^{12} \\ &+ 101q^{13} + \underline{135}q^{14} + 176q^{15} + 231q^{16} \\ &+ 297q^{17} + 385q^{18} + \overline{490}q^{19} \\ &+ 627q^{20} + 792q^{21} + 1002q^{22} \\ &+ \dots + p(200)q^{200} + \dots \end{aligned}$$

(4)

- Cases  $5n + 4$  and  $7n + 5$  are flagged in (4).
- Of course, it is easier to (heuristically) confirm than find these fine examples of **Mathematics: the science of patterns**\*

\*Keith Devlin's 1997 book.

## IS HARD or EASY BETTER?

A modern computationally driven question is *How hard is  $p(n)$  to compute?*

- In **1900**, it took the father of combinatorics, Major Percy MacMahon (1854–1929), months to compute  $p(200)$  using recursions developed from (3).
- By **2000**, *Maple* would produce  $p(200)$  in seconds if one simply demands the 200'th term of the Taylor series. A few years earlier it required being careful to compute the series for  $\prod_{n \geq 1} (1 - q^n)$  *first* and *then* the series for the *reciprocal* of that series!
- This baroque event is occasioned by *Euler's pentagonal number theorem*

$$\prod_{n \geq 1} (1 - q^n) = \sum_{n = -\infty}^{\infty} (-1)^n q^{(3n+1)n/2}.$$

- The reason is that, if one takes the series for (3), the software has to deal with **200** terms on the bottom. But the series for  $\prod_{n \geq 1} (1 - q^n)$ , has only to handle the **23** non-zero terms in series in the pentagonal number theorem.
- If introspection fails, we can find the *pentagonal numbers* occurring above in Sloane and Plouffe's on-line '**Encyclopedia of Integer Sequences**': [www.research.att.com/personal/njas/sequences/eisonline.html](http://www.research.att.com/personal/njas/sequences/eisonline.html).
- This ex post facto algorithmic analysis can be used to facilitate independent student discovery of the pentagonal number theorem, and like results.

- The difficulty of estimating the size of  $p(n)$  analytically—so as to avoid enormous or unattainable computational effort—led to some marvellous mathematical advances\*.
- The corresponding ease of computation may now act as a retardant to insight.
- New mathematics is discovered only when prevailing tools run totally out of steam.
- This raises a caveat against mindless computing:

*Will a student or researcher discover structure when it is easy to compute without needing to think about it? Today, she may thoughtlessly compute  $p(500)$  which a generation ago took much, much pain and insight.*

\*By researchers including Hardy and Ramanujan, and Rademacher

## CONVEX CONJUGATES and NMR(MRI)

The *Hoch and Stern information measure*, or *neg-entropy*, is defined in complex  $n$ -space by

$$H(z) = \sum_{j=1}^n h(z_j/b),$$

where  $h$  is convex and given (for scaling  $b$ ) by:

$$h(z) \triangleq |z| \ln \left( |z| + \sqrt{1 + |z|^2} \right) - \sqrt{1 + |z|^2}$$

for quantum theoretic (NMR) reasons.

- Recall the *Fenchel-Legendre conjugate*

$$f^*(y) := \sup_x \langle y, x \rangle - f(x).$$

- Our *symbolic convex analysis* package (stored at [www.cecm.sfu.ca/projects/CCA/](http://www.cecm.sfu.ca/projects/CCA/)) produced:

$$h^*(z) = \cosh(|z|).$$

- Compare the fundamental *Boltzmann-Shannon entropy*:

$$(z \ln z - z)^* = \exp(z).$$

★ I'd never have tried by hand!

- Knowing 'closed forms' helps:

$$(\exp \exp)^*(y) = y \ln(y) - y \{W(y) + W(y)^{-1}\}$$

where *Maple* or *Mathematica* recognize the complex *Lambert W* function

$$W(x)e^{W(x)} = x.$$

Thus, the conjugate's series is

$$-1 + (\ln(y) - 1)y - \frac{1}{2}y^2 + \frac{1}{3}y^3 - \frac{3}{8}y^4 + \frac{8}{15}y^5 + O(y^6)$$

## WHAT is ENTROPY?

*Despite the narrative force that the concept of entropy appears to evoke in everyday writing, in scientific writing entropy remains a thermodynamic quantity and a mathematical formula that numerically quantifies disorder. When the American scientist Claude Shannon found that the mathematical formula of Boltzmann defined a useful quantity in information theory, he hesitated to name this newly discovered quantity entropy because of its philosophical baggage. The mathematician John Von Neumann encouraged Shannon to go ahead with the name entropy, however, since “no one knows what entropy is, so in a debate you will always have the advantage.” (The American Heritage Book of English Usage, p. 158).*

- **19C:** Boltzmann—thermodynamic disorder
- **20C:** Shannon—information uncertainty
- **21C:** JMB—potentials with superlinear growth



Information theoretic characterizations abound.  
A nice one is:

**Theorem** Up to a positive scalar multiple

$$H(\vec{p}) = - \sum_{k=1}^N p_k \log p_k$$

is the unique continuous function on finite probabilities such that

a. Uncertainly grows:

$$H \left( \overbrace{\left( \frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n} \right)}^n \right)$$

increases with  $n$ .

b. Subordinate choices are respected: for distributions  $\vec{p}_1$  and  $\vec{p}_2$  and  $0 < p < 1$ ,

$$H(p\vec{p}_1, (1-p)\vec{p}_2) = p H(\vec{p}_1) + (1-p) H(\vec{p}_2).$$

## SOME FOURIER INTEGRALS

Recall the *sinc* function

$$\operatorname{sinc}(x) := \frac{\sin(x)}{x}.$$

Consider, the seven highly oscillatory integrals below.\*

$$I_1 := \int_0^\infty \operatorname{sinc}(x) dx = \frac{\pi}{2},$$

$$I_2 := \int_0^\infty \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) dx = \frac{\pi}{2},$$

$$I_3 := \int_0^\infty \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \operatorname{sinc}\left(\frac{x}{5}\right) dx = \frac{\pi}{2},$$

...

$$I_6 := \int_0^\infty \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{11}\right) dx = \frac{\pi}{2},$$

$$I_7 := \int_0^\infty \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{13}\right) dx = \frac{\pi}{2}.$$

\*These are hard to compute accurately numerically.

However,

$$\begin{aligned} I_8 &:= \int_0^\infty \operatorname{sinc}(x) \operatorname{sinc}\left(\frac{x}{3}\right) \cdots \operatorname{sinc}\left(\frac{x}{15}\right) dx \\ &= \frac{467807924713440738696537864469}{935615849440640907310521750000} \pi \\ &\approx 0.49999999999992646\pi. \end{aligned}$$

► When a researcher, using a well-known computer algebra package, checked this he – and the makers – concluded there was a “bug” in the software. Not so!

◇ Our analysis, via Parseval’s theorem, links the integral

$$I_N := \int_0^\infty \operatorname{sinc}(a_1 x) \operatorname{sinc}(a_2 x) \cdots \operatorname{sinc}(a_N x) dx$$

with the volume of the polyhedron  $P_N$  given by

$$P_N := \left\{ x : \left| \sum_{k=2}^N a_k x_k \right| \leq a_1, |x_k| \leq 1, 2 \leq k \leq N \right\}.$$

where  $x := (x_2, x_3, \dots, x_N)$ .

If we let

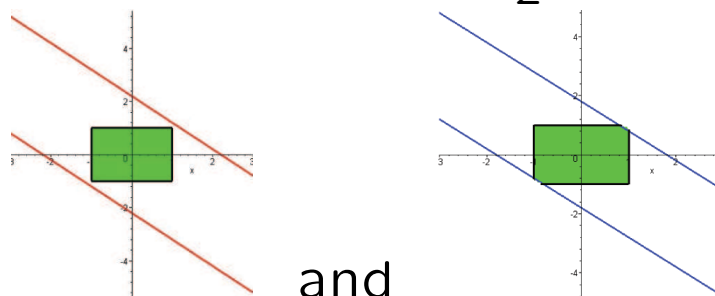
$$C_N := \{(x_2, x_3, \dots, x_N) : -1 \leq x_k \leq 1, 2 \leq k \leq N\},$$

then

$$I_N = \frac{\pi \text{Vol}(P_N)}{2a_1 \text{Vol}(C_N)}.$$

► Thus, the value drops precisely when the constraint  $\sum_{k=2}^N a_k x_k \leq a_1$  becomes *active* and bites the hypercube  $C_N$ . That occurs when  $\sum_{k=2}^N a_k > a_1$ .

In the above,  $\frac{1}{3} + \frac{1}{5} + \dots + \frac{1}{13} < 1$ , but on addition of the term  $\frac{1}{15}$ , the sum exceeds 1, the volume drops, and  $I_N = \frac{\pi}{2}$  no longer holds.



- A somewhat cautionary example for too enthusiastically inferring patterns from seemingly compelling computation.

## **ENIAC: Integrator and Calculator**

**SIZE/WEIGHT:** ENIAC had 18,000 vacuum tubes, 6,000 switches, 10,000 capacitors, 70,000 resistors, 1,500 relays, was 10 feet tall, occupied 1,800 square feet and weighed 30 tons.



**SPEED/MEMORY:** A 1.5GHz Pentium does 3 million adds/sec. ENIAC did 5,000 — 1,000 times faster than any earlier machine. The first stored-memory computer, ENIAC could store 200 digits.

**ARCHITECTURE:** Data flowed from one accumulator to the next, and after each accumulator finished a calculation, it communicated its results to the next in line.

The accumulators were connected to each other manually.

- The 1949 computation of  $\pi$  to 2,037 places took 70 hours.
- It would have taken roughly 100,000 ENIACs to store the Smithsonian's picture!

## BERLINSKI

*The computer has in turn changed the very nature of mathematical experience, suggesting for the first time that mathematics, like physics, may yet become an empirical discipline, a place where things are discovered because they are seen.*

David Berlinski, "Ground Zero: A Review of *The Pleasures of Counting*, by T. W. Koerner," 1997.

- As all sciences rely more on 'dry experiments', via computer simulation, the boundary between physics (e.g., *string theory*) and mathematics (e.g., by *experiment*) is delightfully blurred.
- An early exciting example is provided by **gravitational boosting**.

... and ...

*The body of mathematics to which the calculus gives rise embodies a certain swashbuckling style of thinking, at once bold and dramatic, given over to large intellectual gestures and indifferent, in large measure, to any very detailed description of the world.*

*It is a style that has shaped the physical but not the biological sciences, and its success in Newtonian mechanics, general relativity and quantum mechanics is among the miracles of mankind. But the era in thought that the calculus made possible is coming to an end. Everyone feels this is so and everyone is right.*

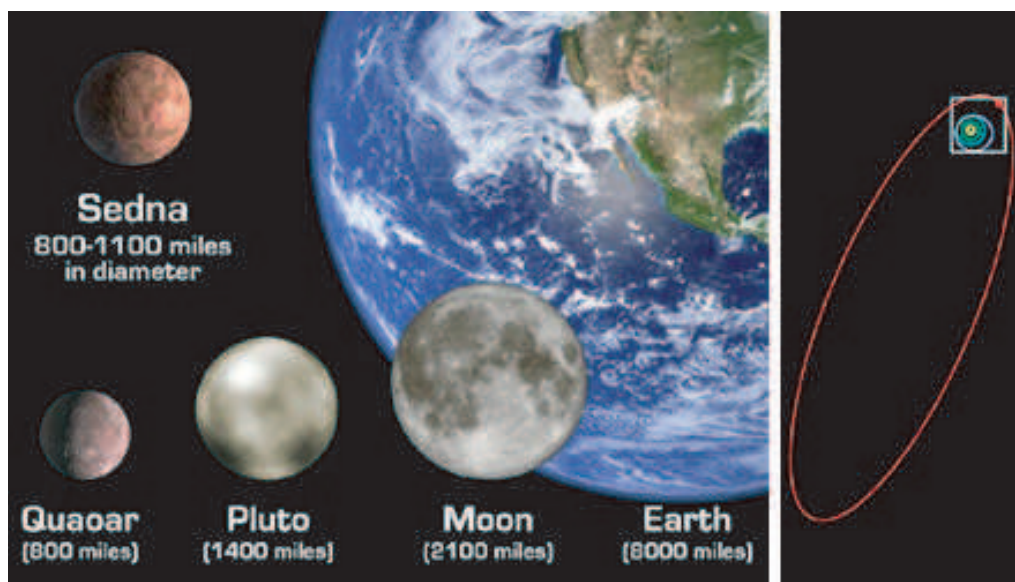


## GRAVITATIONAL BOOSTING

“The Voyager Neptune Planetary Guide” (JPL Publication 89–24) has an excellent description of Michael Minovitch’ computational and unexpected discovery of *gravitational boosting* (also known as slingshot magic) at the Jet Propulsion Laboratory in 1961.

The article starts by quoting Arthur C. Clarke

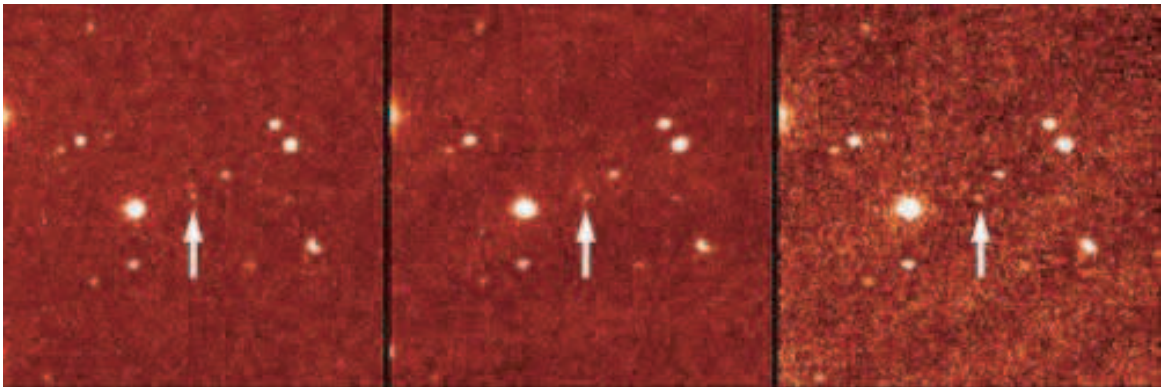
*“Any sufficiently advanced technology is indistinguishable from magic.”*



**Sedna And Friends in 2004**

Until he showed *Hohmann transfer ellipses* were not least energy paths to the outer planets:

**“most planetary mission designers considered the gravity field of a target planet to be somewhat of a nuisance, to be cancelled out, usually by onboard Rocket thrust.”**



- Without a boost from the orbits of [Saturn](#), [Jupiter and Uranus](#), the Earth-to-Neptune Voyager mission (achieved in 1989 in around a decade) would have taken over 30 years!
- We would still be waiting; longer to see Sedna confirmed (8 billion miles away—3 times further than Pluto).

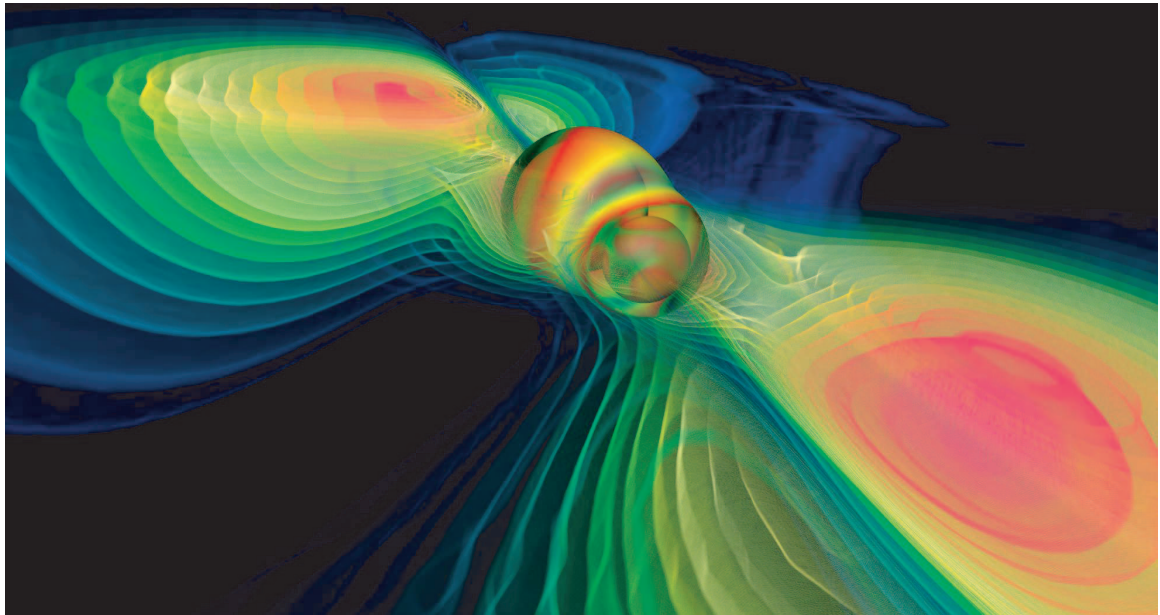
## LIGO: MATH and the COSMOS

**Einstein's theory of general relativity** describes how massive bodies curve space and time; it realizes gravity as movement of masses along shortest paths in curved space-time.

- A subtle mathematical inference is that relatively accelerating bodies will produce ripples on the curved space-time surface, propagating at the speed of light: **gravitational waves**.

These extraordinarily weak cosmic signals hold the key to a new era of astronomy *if only* we can build detectors and untangle the mathematics to interpret them. The signal to noise ratio is tiny!

**LIGO**, the [Laser Interferometer Gravitational-Wave Observatory](#), is such a developing US gravitational wave detector.



**One of the first 3D simulations of the gravitational waves arising when two black holes collide**

- Only recently has the computational power existed to realise such simulations, on computers such as at WestGrid.

## PI and FRIENDS

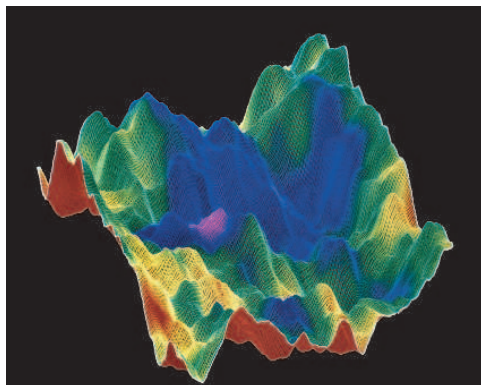
**A:** (A quartic algorithm.) Set  $a_0 = 6 - 4\sqrt{2}$  and  $y_0 = \sqrt{2} - 1$ . Iterate

$$y_{k+1} = \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}}$$

$$a_{k+1} = a_k(1 + y_{k+1})^4 - 2^{2k+3}y_{k+1}(1 + y_{k+1} + y_{k+1}^2)$$

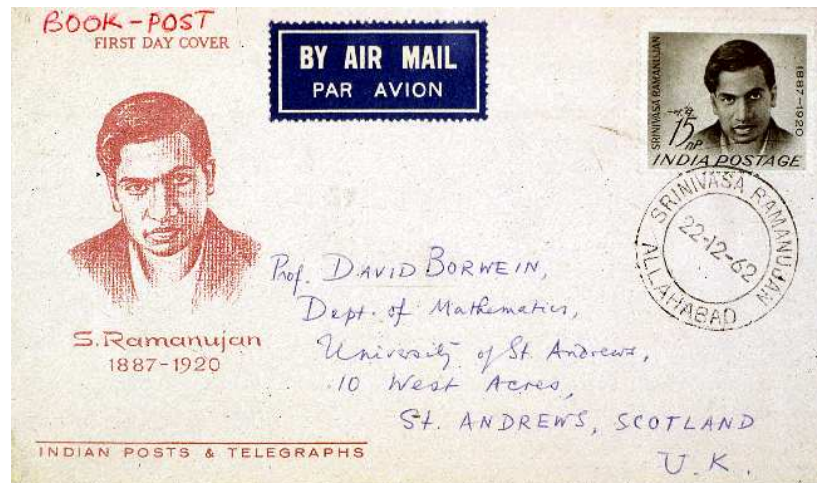
Then  $a_k$  converges *quartically* to  $1/\pi$ .

- Used since 1986, with Salamin-Brent scheme, by Bailey, Kanada (Tokyo).



**A random  
walk on  
a million  
digits of  $\pi$**

# RAMANUJAN (1887-1920)



Ramanujan (**1910**) found remarkable series, barely known (nor fully proven) until recently when his *Notebooks* were fully edited:

$$(5) \frac{1}{\pi} = \frac{2\sqrt{2}}{9801} \sum_{k=0}^{\infty} \frac{(4k)! (1103 + 26390k)}{(k!)^4 396^{4k}}$$

Each term adds *eight* correct digits. When Gosper used (5) to compute 17 million digits of (the continued fraction for)  $\pi$  in 1985, **this concluded the first proof of (5)!**

## BACK to THE FUTURE

► In 1997, Kanada computed over 51 billion digits on a Hitachi supercomputer (18 iterations, 25 hrs on  $2^{10}$  cpu's), and  $2^{36}$  digits in April 1999.

► In December 2002, Kanada computed  $\pi$  to over **1.24 trillion decimal digits**. His team first computed  $\pi$  in hexadecimal (base 16) to 1,030,700,000,000 places, using the following two arctangent relations:

$$\pi = 48 \tan^{-1} \frac{1}{49} + 128 \tan^{-1} \frac{1}{57} - 20 \tan^{-1} \frac{1}{239} + 48 \tan^{-1} \frac{1}{110443}$$

$$\pi = 176 \tan^{-1} \frac{1}{57} + 28 \tan^{-1} \frac{1}{239} - 48 \tan^{-1} \frac{1}{682} + 96 \tan^{-1} \frac{1}{12943}$$

► Kanada verified the results of these two computations agreed (also with 'BBP'), and then converted the hex digit sequence to decimal and back.

- A billion ( $2^{30}$ ) digit computation has been performed on a single Pentium II PC in under 9 days.

- 50 billionth decimal digit of  $\pi$  and  $1/\pi$  is **042** !

- ★ And after 17 billion digits 0123456789 has finally appeared (Brouwer's famous intuitionist example *now* converges!)

► Kanada's estimate of time to run the same FFT/Karatsuba-based  $\pi$  algorithm on a serial machine: "*infinite*".

Details at: [www.cecm.sfu.ca/personal/jborwein/pi\\_cover.html](http://www.cecm.sfu.ca/personal/jborwein/pi_cover.html).



## 'PENTIUM FARMING' for BITS

**B:** Bailey, P. Borwein and Plouffe (1996) discovered a series for  $\pi$  (and other *polylogarithmic constants*) which allows one to compute hex-digits of  $\pi$  *without* computing prior digits.

► This needs little memory and no multiple precision. Run time grows only slightly faster than linearly:

► The key, found by 'PSLQ' (below) is:

$$\pi = \sum_{k=0}^{\infty} \left(\frac{1}{16}\right)^k \left(\frac{4}{8k+1} - \frac{2}{8k+4} - \frac{1}{8k+5} - \frac{1}{8k+6}\right)$$

- Knowing an algorithm would follow they spent months hunting for such a formula.
- Once found it is easy to prove in *Mathematica*, *Maple* or by hand—and is used in the g95 FORTRAN compiler for transcendental function evaluations.

A most successful case of

**REVERSE  
MATHEMATICAL  
ENGINEERING**

► (Sept 97) Fabrice Bellard (INRIA) used a variant formula to compute 152 binary digits of  $\pi$ , starting at the *trillionth position* ( $10^{12}$ ). This took 12 days on 20 work-stations working in parallel over the Internet.

► (August 98) Colin Percival (SFU, age 17) finished a similar ‘embarrassingly parallel’ computation of *five trillionth bit* (using 25 machines at about 10 times the speed). In *Hex*:

07E45733CC790B5B5979

The binary digits of  $\pi$  starting at the 40 trillionth place are

00000111110011111.

► (September 2000) The quadrillionth bit is '0' (used 250 cpu years on 1734 machines in 56 countries). From the 999,999,999,999,997th bit of  $\pi$  one has:

111000110001000010110101100000110

★ One of the largest computations ever!

Bailey and Crandall (2001) make a reasonable, hence very hard conjecture, about the **uniform distribution of a related chaotic dynamical system**. This conjecture implies:

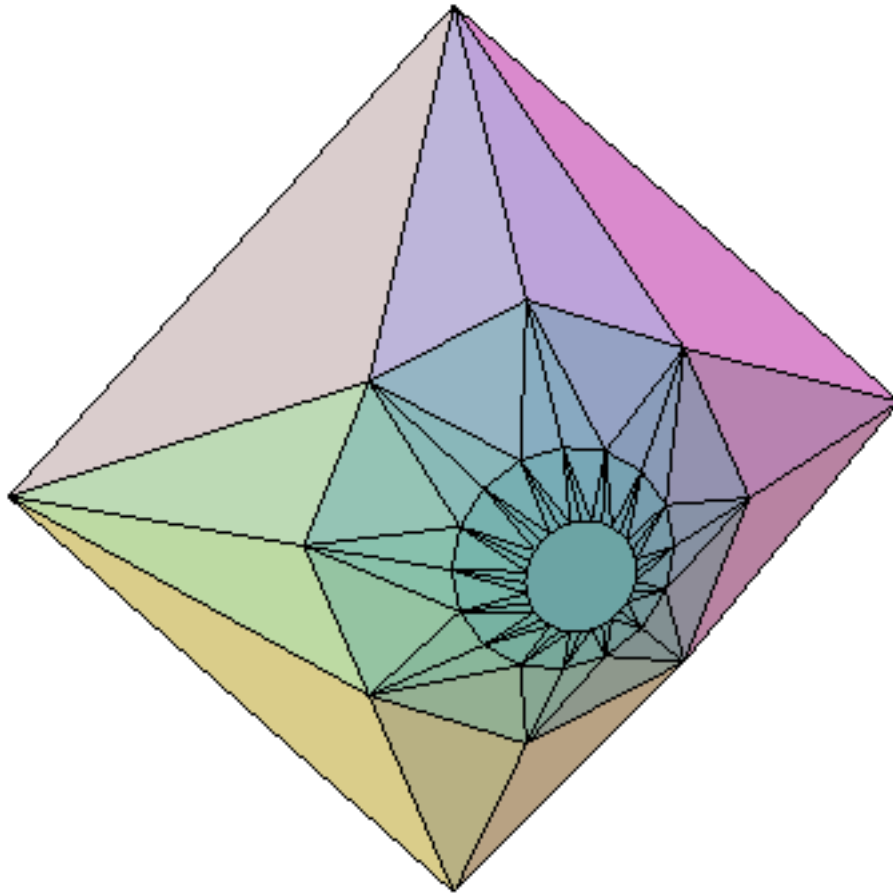
*Existence of a 'BBP' formula base  $b$  for  $\alpha$  ensures the normality base  $b$  of  $\alpha$ .*

For  $\log 2$  the dynamical system is

$$x_{n+1} \leftrightarrow 2\left(x_n + \frac{1}{n}\right) \pmod{1},$$

See [www.sciencenews.org/20010901/bob9.asp](http://www.sciencenews.org/20010901/bob9.asp) .

## A MISLEADING PICTURE



**Polytopic except at one point?**

## DISJOINT GENERA

**Theorem 1** *There are at most 19 integers not of the form of  $xy + yz + xz$  with  $x, y, z \geq 1$ .*

*The only non-square-free are 4 and 18. The first 16 square-free are*

1, 2, 6, 10, 22, 30, 42, 58, 70, 78, 102

130, 190, **210**, 330, 462.

*which correspond to “discriminants with one quadratic form per genus”.*

- If the 19th exists, it is greater than  $10^{11}$  which the Generalized *Riemann Hypothesis* (GRH)\* excludes.

► *Matlab* was the road to proof and showed the hazards of (not) using *Sloane's Encyclopedia*.

\*A million dollar *Millennium Problem*.

## A FULL EXAMPLE—LOG-CONCAVITY

Consider the *unsolved* **Problem 10738** in the 1999 *American Mathematical Monthly*:

**Problem:** For  $t > 0$  let

$$m_n(t) = \sum_{k=0}^{\infty} k^n \exp(-t) \frac{t^k}{k!}$$

be the  $n$ th moment of a *Poisson distribution* with parameter  $t$ . Let  $\mathbf{c}_n(t) = \mathbf{m}_n(t)/\mathbf{n!}$ . Show

- a)  $\{m_n(t)\}_{n=0}^{\infty}$  is log-convex\* for all  $t > 0$ .
- b)  $\{c_n(t)\}_{n=0}^{\infty}$  is not log-concave for  $t < 1$ .
- c\*)  $\{c_n(t)\}_{n=0}^{\infty}$  is log-concave for  $t \geq 1$ .

\*A sequence  $\{a_n\}$  is *log-convex* if  $a_{n+1}a_{n-1} \geq a_n^2$ , for  $n \geq 1$  and log-concave when the sign is reversed.

**Solution.** (a) Neglecting the factor of  $\exp(-t)$  as we may, this reduces to

$$\sum_{k,j \geq 0} \frac{(jk)^{n+1} t^{k+j}}{k! j!} \leq \sum_{k,j \geq 0} \frac{(jk)^n t^{k+j}}{k! j!} k^2 = \sum_{k,j \geq 0} \frac{(jk)^n t^{k+j}}{k! j!} \frac{k^2 + j^2}{2},$$

and this now follows from  $2jk \leq k^2 + j^2$ .

(b) As

$$m_{n+1}(t) = t \sum_{k=0}^{\infty} (k+1)^n \exp(-t) \frac{t^k}{k!},$$

on applying the binomial theorem to  $(k+1)^n$ , we see that  $m_n(t)$  satisfies the recurrence

$$m_{n+1}(t) = t \sum_{k=0}^n \binom{n}{k} m_k(t), \quad m_0(t) = 1.$$

In particular for  $t = 1$ , we obtain the sequence

$$1, 1, 2, 5, 15, 52, 203, 877, 4140 \dots$$

- These are the *Bell numbers* as was discovered by consulting *Sloane's Encyclopedia*.  
[www.research.att.com/~njas/sequences/index.html](http://www.research.att.com/~njas/sequences/index.html)
- Sloane can also tell us that, for  $t = 2$ , we have the generalized Bell numbers, and gives the exponential generating functions.\*

► Inter alia, an explicit computation shows that

$$t \frac{1+t}{2} = c_0(t) c_2(t) \leq c_1(t)^2 = t^2$$

exactly if  $t \geq 1$ , which completes (b).

Also, preparatory to the next part, a simple calculation shows that

$$(6) \quad \sum_{n \geq 0} c_n u^n = \exp(t(e^u - 1)).$$

\*The Bell numbers were known earlier to Ramanujan — an example of *Stigler's Law of Eponymy!*



(c\*)<sup>\*</sup> We appeal to a recent theorem due to E. Rodney Canfield,<sup>†</sup> which proves the lovely and quite difficult result below.

**Theorem 2** *If a sequence  $1, b_1, b_2, \dots$  is non-negative and log-concave then so is the sequence  $1, c_1, c_2, \dots$  determined by the generating function equation*

$$\sum_{n \geq 0} c_n u^n = \exp \left( \sum_{j \geq 1} b_j \frac{u^j}{j} \right).$$

Using equation (6) above, we apply this to the sequence  $b_j = t/(j - 1)!$  which is log-concave exactly for  $t \geq 1$ . **QED**

\*The ‘\*’ indicates this was the unsolved component.

†A search in 2001 on *MathSciNet* for “Bell numbers” since 1995 turned up 18 items. This paper showed up as number 10. Later, *Google* found it immediately!

- It transpired that the given solution to (c) was the only one received by the *Monthly*.
  - ▶ This is quite unusual.
- The reason might well be that it relied on the following sequence of steps:

(??) ⇒ Computer Algebra System ⇒ Interface

⇒ Search Engine ⇒ Digital Library

⇒ Hard New Paper ⇒ **Answer**

★ Now if only we could automate this!

## ANOTHER CONCRETE SYNOPSIS

I illustrate some of the mathematical challenges with a second specific problem, proposed in the *American Mathematical Monthly* (November, 2000), as described in [6].

**10832.** *Donald E. Knuth, Stanford University, Stanford, CA.* Evaluate

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

**1.** A very rapid Maple computation yielded  $-0.08406950872765600\dots$  as the first 16 digits of the sum.

**2.** The Inverse Symbolic Calculator has a ‘smart lookup’ feature\* that replied that this was probably  $-\frac{2}{3} - \zeta(\frac{1}{2})/\sqrt{2\pi}$ .

\*Alternatively, a sufficiently robust integer relation finder could be used.

3. Ample experimental confirmation was provided by checking this to 50 digits. Thus within minutes we *knew* the answer.

4. As to why? A clue was provided by the surprising speed with which Maple computed the slowly convergent infinite sum.

The package clearly knew something the user did not. Peering under the covers revealed that it was using the *LambertW* function,  $W$ , which is the inverse of  $w = z \exp(z)$ .\*

\*A search for 'Lambert W function' on MathSciNet provided 9 references – all since 1997 when the function appears named for the first time in Maple and Mathematica.

5. The presence of  $\zeta(1/2)$  and standard Euler-MacLaurin techniques, using Stirling's formula (as might be anticipated from the question), led to

$$(7) \quad \sum_{k=1}^{\infty} \left( \frac{1}{\sqrt{2\pi k}} - \frac{1}{\sqrt{2}} \frac{(\frac{1}{2})_{k-1}}{(k-1)!} \right) = \frac{\zeta(\frac{1}{2})}{\sqrt{2\pi}},$$

where the binomial coefficients in (7) are those of  $\frac{1}{\sqrt{2-2z}}$ .

Now (7) is a formula Maple can 'prove'.

6. It remains to show

$$(8) \quad \sum_{k=1}^{\infty} \left( \frac{k^k}{k! e^k} - \frac{1}{\sqrt{2}} \frac{(\frac{1}{2})_{k-1}}{(k-1)!} \right) = -\frac{2}{3}.$$

7. Guided by the presence of  $W$ , and its series

$$W(z) = \sum_{k=1}^{\infty} \frac{(-k)^{k-1} z^k}{k!},$$

an appeal to Abel's limit theorem lets one deduce the need to evaluate

$$(9) \quad \lim_{z \rightarrow 1} \left( \frac{d}{dz} W\left(-\frac{z}{e}\right) + \frac{1}{\sqrt{2-2z}} \right) = \frac{2}{3}.$$

Again Maple happily does know (9).

8. Of course, this all took a *fair* amount of human mediation and insight.

## KUHN

*The issue of paradigm choice can never be unequivocally settled by logic and experiment alone.*

...

*in these matters neither proof nor error is at issue. The transfer of allegiance from paradigm to paradigm is a conversion experience that cannot be forced.*

- In *Who Got Einstein's Office?* ([Beurling](#))

*And Max Planck, surveying his own career in his Scientific Autobiography, sadly remarked that 'a new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it.'*

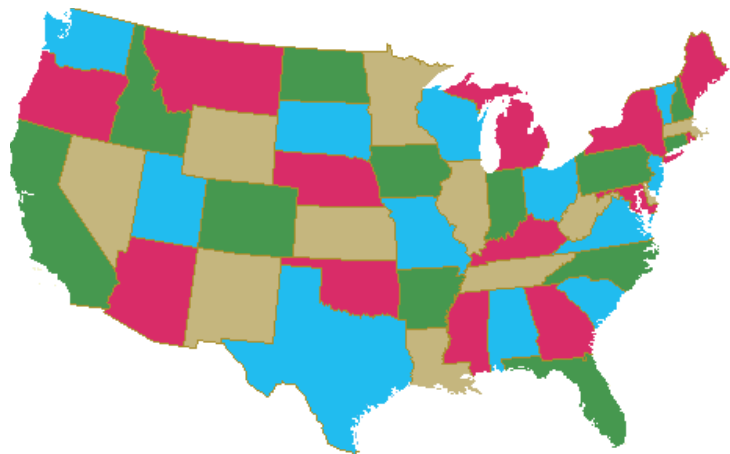
## A PARAPHRASE of HERSH

► Whatever the outcome of these developments, **mathematics is and will remain a uniquely human undertaking**. Indeed Reuben Hersh's arguments for a humanist philosophy of mathematics, as paraphrased below, become more convincing in our setting:

1. *Mathematics is human*. It is part of and fits into human culture. It does not match Frege's concept of an abstract, timeless, tenseless, objective reality.
2. *Mathematical knowledge is fallible*. As in science, mathematics can advance by making mistakes and then correcting or even re-correcting them. The "fallibilism" of mathematics is brilliantly argued in Lakatos' *Proofs and Refutations*.



3. *There are different versions of proof or rigor.* Standards of rigor can vary depending on time, place, and other things. The use of computers in formal proofs, exemplified by the computer-assisted proof of the **four color theorem** in 1977 (1997), is just one example of an emerging nontraditional standard of rigor.



4. *Empirical evidence, numerical experimentation and probabilistic proof all can help us decide what to believe in mathematics.* Aristotelian logic isn't necessarily always the best way of deciding.

5. *Mathematical objects are a special variety of a social-cultural-historical object.* Contrary to the assertions of certain post-modern detractors, mathematics cannot be dismissed as merely a new form of literature or religion. Nevertheless, many mathematical objects can be seen as shared ideas, like Moby Dick in literature, or the Immaculate Conception in religion.

► From “Fresh Breezes in the Philosophy of Mathematics”, *American Mathematical Monthly*, August-Sept 1995, 589–594.

► The recognition that “quasi-intuitive” analogies may be used to gain insight in mathematics can assist in the learning of mathematics.

And honest mathematicians will acknowledge their role in discovery as well. We should look forward to what the future will bring.

## HILBERT

*Moreover a mathematical problem should be difficult in order to entice us, yet not completely inaccessible, lest it mock our efforts. It should be to us a guidepost on the mazy path to hidden truths, and ultimately a reminder of our pleasure in the successful solution.*

...

*Besides it is an error to believe that rigor in the proof is the enemy of simplicity. (David Hilbert)*

- In his '23' "Mathematische Probleme" lecture to the Paris International Congress, 1900 (see Ben Yandell's fine account in *The Honors Class*, AK Peters, 2002).

## CHAITIN

*I believe that elementary number theory and the rest of mathematics should be pursued more in the spirit of experimental science, and that you should be willing to adopt new principles. I believe that Euclid's statement that an axiom is a self-evident truth is a big mistake\*. The Schrödinger equation certainly isn't a self-evident truth! **And the Riemann Hypothesis isn't self-evident either, but it's very useful.** A physicist would say that there is ample experimental evidence for the Riemann Hypothesis and would go ahead and take it as a working assumption.*

\*There is no evidence that Euclid ever made such a statement. However, the statement does have an undeniable emotional appeal.

*In this case, we have ample experimental evidence for the truth of our identity and we may want to take it as something more than just a working assumption. We may want to introduce it formally into our mathematical system.*

- Greg Chaitin (1994). A like article is in press in the *Mathematical Intelligencer*.



**A tangible Riemann surface for  $W$**

## CARATHÉODORY and CHRÉTIEN

*I'll be glad if I have succeeded in impressing the idea that it is not only pleasant to read at times the works of the old mathematical authors, but this may occasionally be of use for the actual advancement of science.*

- Constantin Carathéodory, at an MAA meeting in 1936 (retro-digital data-mining?).

*A proof is a proof. What kind of a proof? It's a proof. A proof is a proof. And when you have a good proof, it's because it's proven.*

(Jean Chrétien, 2002)

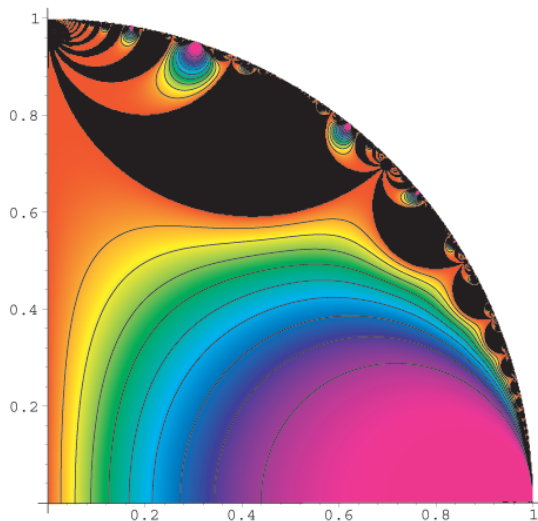
- The Prime Minister, explaining how Canada would determine if Iraq had WMDs, sounds a lot like Bertrand Russell!

## GAUSS

► In Boris Stoicheff's often enthralling biography of Herzberg\*, Gauss is recorded as writing:

*It is not knowledge, but the act of learning, not possession but the act of getting there which generates the greatest satisfaction.*

**Fractal similarity in Gauss' discovery of modular functions**



\*Gerhard Herzberg (1903-99) fled Germany for Saskatchewan in 1935 and won the 1971 Chemistry Nobel.

## A FEW CONCLUSIONS

- The traditional deductive accounting of Mathematics is a largely ahistorical caricature.\*
- Mathematics is primarily about secure knowledge not proof, and the aesthetic is central.
- Proofs are often out of reach — understanding, even certainty, is not.
- Packages can make concepts accessible (Linear relations, Galois theory, Groebner bases).
- While progress is made “one funeral at a time” (Niels Bohr), “you can’t go home again” (Thomas Wolfe).

\*Quotations are at [jborwein/quotations.html](http://jborwein/quotations.html)



# HOW NOT TO EXPERIMENT



## Pooh Math

'Guess and Check'  
while

Aiming Too High

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3. D.H. Bailey and J.M. Borwein, “Experimental Mathematics: Recent Developments and Future Outlook,” pp, 51-66 in Vol. I of *Mathematics Unlimited — 2001 and Beyond*, B. Engquist & W. Schmid (Eds.), Springer-Verlag, 2000. [CECM 99:143]

\*All references are at [www.cecm.sfu.ca/preprints](http://www.cecm.sfu.ca/preprints).

4. J. Dongarra, F. Sullivan, “The top 10 algorithms,” *Computing in Science & Engineering*, **2** (2000), 22–23.  
(See [personal/jborwein/algorithms.html](http://personal.jborwein/algorithms.html).)
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6. J.M. Borwein and D.H. Bailey), **Mathematics by Experiment: Plausible Reasoning in the 21st Century**, and **Experimentation in Mathematics: Computational Paths to Discovery**, (with R. Girgensohn,) AK Peters Ltd, 2003-04.  
  
▶ The web site is at [www.expmath.info](http://www.expmath.info)

## APPENDIX: INTEGER RELATIONS

### The USES of LLL and PSLQ

► A vector  $(x_1, x_2, \dots, x_n)$  of reals *possesses an integer relation* if there are integers  $a_i$  not all zero with

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

**PROBLEM:** Find  $a_i$  if such exist. If not, obtain lower bounds on the size of possible  $a_i$ .

- ( $n = 2$ ) *Euclid's algorithm* gives solution.
- ( $n \geq 3$ ) Euler, Jacobi, Poincare, Minkowski, Perron, others sought method.
- *First general algorithm* in 1977 by **Ferguson** & Forcade. Since '77: **LLL** (in Maple), HJLS, PSOS, **PSLQ** ('91, *parallel* '99).

► Integer Relation Detection was recently ranked among “the 10 algorithms with the greatest influence on the development and practice of science and engineering in the 20th century.”  
J. Dongarra, F. Sullivan, *Computing in Science & Engineering* 2 (2000), 22–23.

**Also:** Monte Carlo, Simplex, Krylov Subspace, QR Decomposition, Quicksort, ..., FFT, Fast Multipole Method.

## **A. ALGEBRAIC NUMBERS**

Compute  $\alpha$  to sufficiently high precision ( $O(n^2)$ ) and apply LLL to the vector

$$(1, \alpha, \alpha^2, \dots, \alpha^{n-1}).$$

- Solution integers  $a_i$  are coefficients of a polynomial likely satisfied by  $\alpha$ .
- If no relation is found, exclusion bounds are obtained.

## B. FINALIZING FORMULAE

► If we suspect an identity PSLQ is powerful.

- (*Machin's Formula*) We try `lin_dep` on

$$\left[\arctan(1), \arctan\left(\frac{1}{5}\right), \arctan\left(\frac{1}{239}\right)\right]$$

and recover  $[1, -4, 1]$ . That is,

$$\frac{\pi}{4} = 4 \arctan\left(\frac{1}{5}\right) - \arctan\left(\frac{1}{239}\right).$$

[Used on all serious computations of  $\pi$  from 1706 (100 digits) to 1973 (1 million).]

- (*Dase's 'mental' Formula*) We try `lin_dep` on

$$\left[\arctan(1), \arctan\left(\frac{1}{2}\right), \arctan\left(\frac{1}{5}\right), \arctan\left(\frac{1}{8}\right)\right]$$

and recover  $[-1, 1, 1, 1]$ . That is,

$$\frac{\pi}{4} = \arctan\left(\frac{1}{2}\right) + \arctan\left(\frac{1}{5}\right) + \arctan\left(\frac{1}{8}\right).$$

[Used by Dase for 200 digits in 1844.]

## C. ZETA FUNCTIONS

► The *zeta function* is defined, for  $s > 1$ , by

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

• Thanks to *Apéry* (1976) it is well known that

$$S_2 := \zeta(2) = 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k}}$$
$$A_3 := \zeta(3) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}}$$
$$S_4 := \zeta(4) = \frac{36}{17} \sum_{k=1}^{\infty} \frac{1}{k^4 \binom{2k}{k}}$$

► These results *strongly* suggest that

$$\aleph_5 := \zeta(5) / \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^5 \binom{2k}{k}}$$

is a simple rational or algebraic number. Yet, **PSLQ shows**: if  $\aleph_5$  satisfies a polynomial of degree  $\leq 25$  the Euclidean norm of coefficients exceeds  $2 \times 10^{37}$ .

## D. BINOMIAL SUMS and LIN\_DEP

► Any relatively prime integers  $p$  and  $q$  such that

$$\zeta(5) \stackrel{?}{=} \frac{p}{q} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}}$$

have  $q$  astronomically large (as “lattice basis reduction” showed).

► But ... PSLQ yields in *polylogarithms*:

$$\begin{aligned} A_5 &= \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}} = 2\zeta(5) \\ &\quad - \frac{4}{3}L^5 + \frac{8}{3}L^3\zeta(2) + 4L^2\zeta(3) \\ &\quad + 80 \sum_{n>0} \left( \frac{1}{(2n)^5} - \frac{L}{(2n)^4} \right) \rho^{2n} \end{aligned}$$

where  $L := \log(\rho)$  and  $\rho := (\sqrt{5} - 1)/2$ ; with similar formulae for  $A_4, A_6, S_5, S_6$  and  $S_7$ .



- A less known formula for  $\zeta(5)$  due to Koecher suggested generalizations for  $\zeta(7), \zeta(9), \zeta(11) \dots$
- Again the coefficients were found by integer relation algorithms. *Bootstrapping* the earlier pattern kept the search space of manageable size.
- For example, and simpler than Koecher:

$$(10) \quad \zeta(7) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} + \frac{25}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4}$$

► We were able – by finding integer relations for  $n = 1, 2, \dots, 10$  – to encapsulate the formulae for  $\zeta(4n + 3)$  in a single conjectured generating function, (entirely *ex machina*).

► The discovery was:

**Theorem 3** For any complex  $z$ ,

$$\begin{aligned}
 & \sum_{n=0}^{\infty} \zeta(4n+3) z^{4n} \\
 (11) \quad &= \sum_{k=1}^{\infty} \frac{1}{k^3(1-z^4/k^4)} \\
 &= \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k} (1-z^4/k^4)} \prod_{m=1}^{k-1} \frac{1+4z^4/m^4}{1-z^4/m^4}.
 \end{aligned}$$

- The first '=' is easy. The second is quite unexpected in its form!
- $z = 0$  yields Apéry's formula for  $\zeta(3)$  and the coefficient of  $z^4$  is (10).

## HOW IT WAS FOUND

► The first ten cases show (11) has the form

$$\frac{5}{2} \sum_{k \geq 1} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}} \frac{P_k(z)}{(1 - z^4/k^4)}$$

for *undetermined*  $P_k$ ; with abundant data to compute

$$P_k(z) = \prod_{m=1}^{k-1} \frac{1 + 4z^4/m^4}{1 - z^4/m^4}.$$

- We found many reformulations of (11), including a marvellous finite sum:

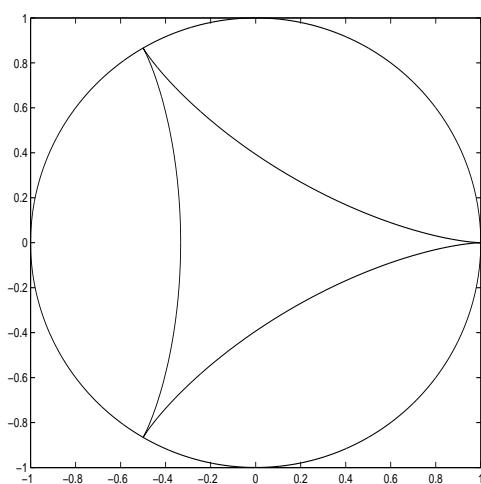
$$(12) \quad \sum_{k=1}^n \frac{2n^2}{k^2} \frac{\prod_{i=1}^{n-1} (4k^4 + i^4)}{\prod_{i=1, i \neq k}^n (k^4 - i^4)} = \binom{2n}{n}.$$

- Obtained via Gosper's (Wilf-Zeilberger type) *telescoping algorithm* after a mistake in an electronic Petri dish ('infty'  $\neq$  'infinity').

► This finite identity was subsequently proved by Almkvist and Granville (*Experimental Math*, 1999) thus finishing the proof of (11) and giving a rapidly converging series for any  $\zeta(4N+3)$  where  $N$  is positive integer.

★ Perhaps shedding light on the irrationality of  $\zeta(7)$ ?

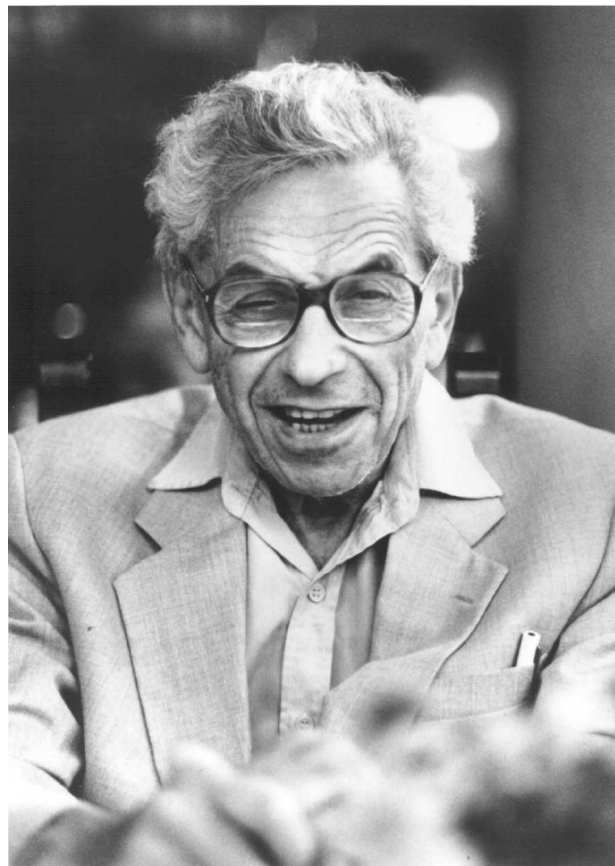
Recall that  $\zeta(2N + 1)$  is not proven irrational for  $N > 1$ . One of  $\zeta(2n + 3)$  for  $n = 1, 2, 3, 4$  is irrational (Rivoal et al).



**Takeya's needle**  
an excellent  
false conjecture

## PAUL ERDŐS (1913-1996)

Paul Erdős, when shown (12) shortly before his death, rushed off.



Twenty minutes later he returned saying he did not know how to prove it but if proven it would have implications for Apéry's result (' $\zeta(3)$  is irrational').

## E. ZAGIER'S CONJECTURE

For  $r \geq 1$  and  $n_1, \dots, n_r \geq 1$ , consider:

$$L(n_1, \dots, n_r; x) := \sum_{0 < m_r < \dots < m_1} \frac{x^{m_1}}{m_1^{n_1} \dots m_r^{n_r}}.$$

Thus

$$L(n; x) = \frac{x}{1^n} + \frac{x^2}{2^n} + \frac{x^3}{3^n} + \dots$$

is the classical *polylogarithm*, while

$$\begin{aligned} L(n, m; x) &= \frac{1}{1^m} \frac{x^2}{2^n} + \left( \frac{1}{1^m} + \frac{1}{2^m} \right) \frac{x^3}{3^n} + \left( \frac{1}{1^m} + \frac{1}{2^m} + \frac{1}{3^m} \right) \frac{x^4}{4^n} \\ &\quad + \dots, \\ L(n, m, l; x) &= \frac{1}{1^l} \frac{1}{2^m} \frac{x^3}{3^n} + \left( \frac{1}{1^l} \frac{1}{2^m} + \frac{1}{1^l} \frac{1}{3^m} + \frac{1}{2^l} \frac{1}{3^m} \right) \frac{x^4}{4^n} + \dots \end{aligned}$$

- The series converge absolutely for  $|x| < 1$  and conditionally on  $|x| = 1$  unless  $n_1 = x = 1$ .

These polylogarithms

$$L(n_r, \dots, n_1; x) = \sum_{0 < m_1 < \dots < m_r} \frac{x^{m_r}}{m_r^{n_r} \dots m_1^{n_1}},$$

are determined uniquely by the **differential equations**

$$\frac{d}{dx} L(\mathbf{n}_r, \dots, n_1; x) = \frac{1}{x} L(\mathbf{n}_r - \mathbf{1}, \dots, n_2, n_1; x)$$

**if**  $n_r \geq 2$  and

$$\frac{d}{dx} L(\mathbf{n}_r, \dots, n_2, n_1; x) = \frac{1}{1-x} L(\mathbf{n}_{r-1}, \dots, n_1; x)$$

**if**  $n_r = 1$  with the *initial conditions*

$$L(n_r, \dots, n_1; 0) = 0$$

for  $r \geq 1$  and

$$L(\emptyset; x) \equiv 1.$$

Set  $\bar{s} := (s_1, s_2, \dots, s_N)$ . Let  $\{\bar{s}\}_n$  denotes concatenation, and  $w := \sum s_i$ .

Then every *periodic* polylogarithm leads to a function

$$L_{\bar{s}}(x, t) := \sum_n L(\{\bar{s}\}_n; x) t^{wn}$$

which solves an algebraic ordinary differential equation in  $x$ , and leads to nice *recurrences*.

**A.** In the simplest case, with  $N = 1$ , the ODE is  $\mathbf{D}_s \mathbf{F} = t^s \mathbf{F}$  where

$$D_s := \left( (1-x) \frac{d}{dx} \right)^1 \left( x \frac{d}{dx} \right)^{s-1}$$

and the solution (by series) is a generalized hypergeometric function:

$$L_{\bar{s}}(x, t) = 1 + \sum_{n \geq 1} x^n \frac{t^s}{n^s} \prod_{k=1}^{n-1} \left( 1 + \frac{t^s}{k^s} \right),$$

as follows from considering  $D_s(x^n)$ .



**B.** Similarly, for  $N = 1$  and negative integers

$$L_{-s}(x, t) := 1 + \sum_{n \geq 1} (-x)^n \frac{t^s}{n^s} \prod_{k=1}^{n-1} \left( 1 + (-1)^k \frac{t^s}{k^s} \right),$$

and  $L_{-1}(2x-1, t)$  solves a hypergeometric ODE.

► Indeed

$$L_{-1}(1, t) = \frac{1}{\beta(1 + \frac{t}{2}, \frac{1}{2} - \frac{t}{2})}.$$

**C.** We may obtain ODEs for eventually periodic Euler sums. Thus,  $L_{-2,1}(x, t)$  is a solution of

$$\begin{aligned} t^6 F &= x^2(x-1)^2(x+1)^2 D^6 F \\ &+ x(x-1)(x+1)(15x^2 - 6x - 7) D^5 F \\ &+ (x-1)(65x^3 + 14x^2 - 41x - 8) D^4 F \\ &+ (x-1)(90x^2 - 11x - 27) D^3 F \\ &+ (x-1)(31x - 10) D^2 F + (x-1) DF. \end{aligned}$$

- This leads to a four-term recursion for  $F = \sum c_n(t)x^n$  with initial values  $c_0 = 1, c_1 = 0, c_2 = t^3/4, c_3 = -t^3/6$ , and the ODE can be simplified.

We are now ready to prove Zagier's conjecture. Let  $F(a, b; c; x)$  denote the *hypergeometric function*. Then:

**Theorem 4 (BBGL)** For  $|x|, |t| < 1$  and integer  $n \geq 1$

$$\begin{aligned}
 & \sum_{n=0}^{\infty} L(\underbrace{3, 1, 3, 1, \dots, 3, 1}_{n\text{-fold}}; x) t^{4n} \\
 (13) \quad & = F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; x\right) \\
 & \times F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; x\right).
 \end{aligned}$$

**Proof.** Both sides of the putative identity start

$$1 + \frac{t^4}{8} x^2 + \frac{t^4}{18} x^3 + \frac{t^8 + 44t^4}{1536} x^4 + \dots$$

and are *annihilated* by the differential operator

$$D_{31} := \left( (1-x) \frac{d}{dx} \right)^2 \left( x \frac{d}{dx} \right)^2 - t^4.$$

**QED**

- Once discovered — and it was discovered after much computational evidence — this can be checked variously in Mathematica or Maple (e.g., in the package *gfun*)!

### Corollary 5 (Zagier Conjecture)

$$(14) \quad \zeta(\underbrace{3, 1, 3, 1, \dots, 3, 1}_{n\text{-fold}}) = \frac{2 \pi^{4n}}{(4n + 2)!}$$

**Proof.** We have

$$F(a, -a; 1; 1) = \frac{1}{\Gamma(1-a)\Gamma(1+a)} = \frac{\sin \pi a}{\pi a}$$

where the first equality comes from Gauss's evaluation of  $F(a, b; c; 1)$ .

Hence, setting  $x = 1$ , in (13) produces

$$\begin{aligned} & F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; 1\right) F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; 1\right) \\ &= \frac{2}{\pi^2 t^2} \sin\left(\frac{1+i}{2}\pi t\right) \sin\left(\frac{1-i}{2}\pi t\right) \\ &= \frac{\cosh \pi t - \cos \pi t}{\pi^2 t^2} = \sum_{n=0}^{\infty} \frac{2\pi^{4n} t^{4n}}{(4n+2)!} \end{aligned}$$

on using the Taylor series of  $\cos$  and  $\cosh$ . Comparing coefficients in (13) ends the proof.

**QED**

- ▶ What other deep Clausen-like hypergeometric factorizations lurk within?
- If one suspects that (5) holds, once one can compute these sums well, it is easy to verify many cases numerically and be entirely convinced.
- ♠ This is the *unique* non-commutative analogue of Euler's evaluation of  $\zeta(2n)$ .