# Experimental Mathematics:

## Finding and Proving Things

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*The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it*. (Jacques Hadamard)

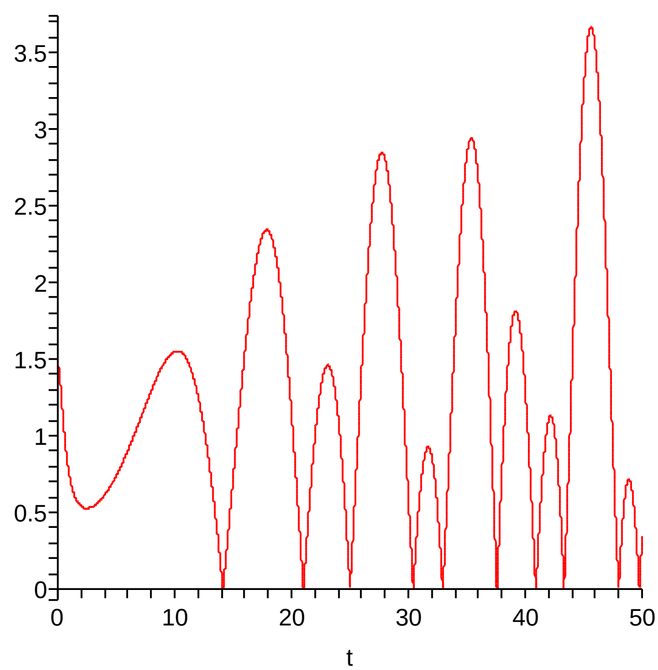
D Drive www.cs.dal.ca/ddrive mathagate

**AK Peters** 2004 **Talk Revised**: 03–20–05

# FINDING vs PROVING THINGS

The second lecture will focus on the differences between *Determining Truths or Proving Theorems.*

We shall explore various of the tools available for deciding what to believe in mathematics, and—using accessible examples—illustrate the rich experimental tool-box mathematicians can now have access to.




**The modulus of $\zeta(1/2+it)$—on the critical line**

★ Let us start with some $\TeX$...

## An Inverse Symbolic Discovery

Donald Knuth* asked for a closed form evaluation of:

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

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

∡ The 'smart lookup' facility in the *Inverse Symbolic Calculator*† rapidly returns

$$0.084069508727655 \approx \frac{2}{3} + \frac{\zeta(1/2)}{\sqrt{2\,\pi}}.$$

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

Arguably we are done. □

*Posed as *MAA Problem* 10832, November 2002.

†At www.cecm.sfu.ca/projects/ISC/ISCmain.html

# A Fuller Account and a Proof

**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

$$-0.084069508727655\ldots$$

as the first 16 digits of the sum.

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

**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.

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

- *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 $w = z \exp(z)$.*

**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

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

where the binomial coefficients in (1) are those of

$$\frac{1}{\sqrt{2-2\,z}}.$$

✓ Now, (1) is a formula *Maple* can 'prove':

*A search in 2000 (2005) for "**Lambert** W" on *MathSciNet* provided 9 (25 ) references – all since 1997 when the function appears named for the first time in *Maple* and *Mathematica*.

**6.** It remains to show

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

**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

$$\lim_{z\to 1}\left(\frac{d}{dz}\mathrm{W}\left(-\frac{z}{e}\right)+\frac{1}{\sqrt{2-2\,z}}\right)=\frac{2}{3}. \qquad (3)$$

✓ Again Maple happily does know (3). □

- Of course, this all took a *fair* amount of human mediation and insight.
- Less if *Maple* had been *taught* to recognize $W$ from its series.

## In the same vein . . .

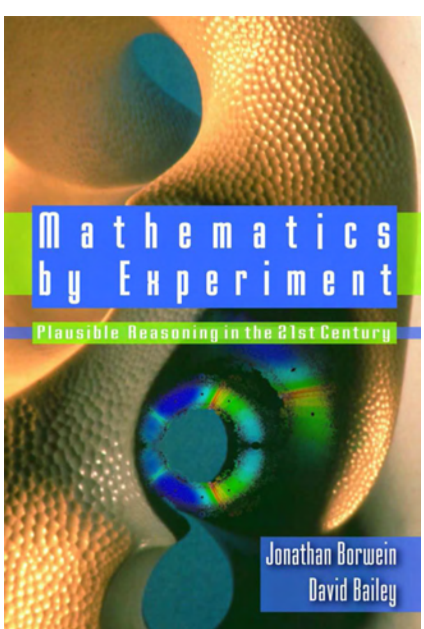
Consider the following two *Euler sum identities* both discovered heuristically.

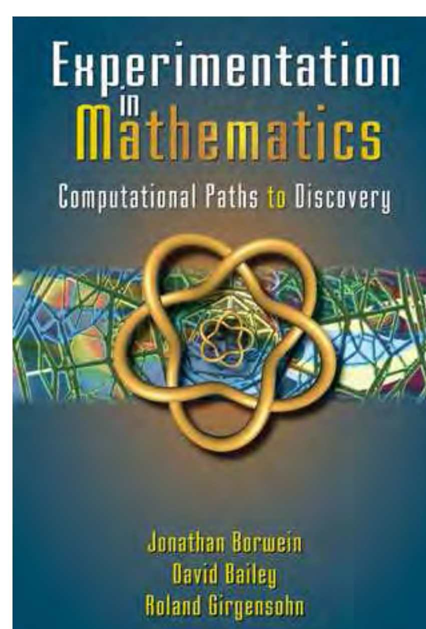
- Both merit quite firm belief—more so than many proofs.

**Why**?

- Only the first warrants significant effort being exerted for its proof.

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



## “Lisez Euler, lisez Euler

**“Lisez Euler, lisez Euler, c’est notre maitre a tous.”** Goldbach precisely formulated by letter the series which sparked Euler’s further investigations into what would become known as the *Zeta-function*.

- These investigations were apparently due to a serendipitous mistake.

  Euler wrote back:

  *When I recently considered further the indicated sums of the last two series in my previous letter, I realized immediately that the same series arose due to a mere writing error, from which indeed the saying goes,* “Had one not erred, one would have achieved less.” (*Si non errasset, fecerat ille minus*).*

*Translation thanks to Martin Matmüller, scientific collaborator of Euler’s *Opera Omnia*, vol. IVA4, Birkhäuser Verlag.

## A FIRST MULTIPLE ZETA VALUE

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

For natural numbers

$$\zeta(i_1, i_2, \ldots, i_k) := \sum_{n_1 > n_2 > \dot{n}_k > 0} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}$$

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

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

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

- This clearly extends to alternating and character sums.

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

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

- MZV's have 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

  – Goldbach's letter conjectured

$$\zeta(3,1) + \zeta(4) = \pi^4/72.$$

- $\zeta(6,2)$ is the lowest weight **'irreducible'**

✓ High precision *fast* $\zeta$*-convolution* (see *EZFace/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:

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

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 was confirmed 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 $n = 1$?

# II. A CHARACTER EULER SUM

Let

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

where $\chi_3$ is the character modulo 3.

Then

$[2b,-3](2N+1,1)$

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

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

- ✓ One first evaluates such sums as integrals

## 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

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

most probably for no good reason.

✓ This seemed more bizarre on an eight digit calculator

Likewise, as spotted by Pierre Lanchon recently

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

while

$$\pi = 11.0010\overline{\mathbf{0100001111110110101}}01000\ldots$$

have 19 bits agreeing in base two—w*ith one read right to left*

- More extended coincidences are almost always contrived ...

- And strong heuristics exist for believing results like the preceding $\zeta$-function and $\pi$ examples.

® But recall the *Skewes number*

$$\int_2^x \frac{dt}{\log t} \geq \pi(x) \quad \text{failure at } (10^{360})$$

and the *Merten Conjecture*

$$\left|\sum_{k=1}^{n} \mu(k)\right| \leq \sqrt{n} \quad \text{failure at } (10^{110})$$

counter-examples.

## HIGH PRECISION FRAUD

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

is valid to 268 places; while

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

is valid to just 12 places.

- Both are actually *transcendental numbers*

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

$$[0, 1, \mathbf{267}, 4, 14, 1, 2, 1, 2, 2, 1, 2, 3, 8, 3, 1]$$

and

$$[0, 1, \mathbf{11}, 14, 4, 1, 1, 1, 3, 1, 295, 4, 4, 1, 5, 17, 7]$$

- 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."

# 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 3 volume compendium contains

$$\sum_{k=1}^{\infty}\sum_{l=1}^{\infty}\frac{1}{k^2\left(k^2-kl+l^2\right)}=\frac{\pi^{\propto}\sqrt{3}}{30}, \qquad (4)$$

where the "$\propto$" is *probably* "4" [volume 1, entry 9, page 750].

★ Integer relation methods suggest that no reasonable value of $\propto$ works

- *Forensic Mathematics* (CSI-Math).
  - what is intended in (4)? There are many such examples (e.g., Lewin on Landen, Fermat's margin)

## SIMON and RUSSELL on INDUCTION

*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.*[13]

*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.*

## FROM 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. After each accumulator finished a calculation, it communicated its results to the next in line

The accumulators were connected to each other manually

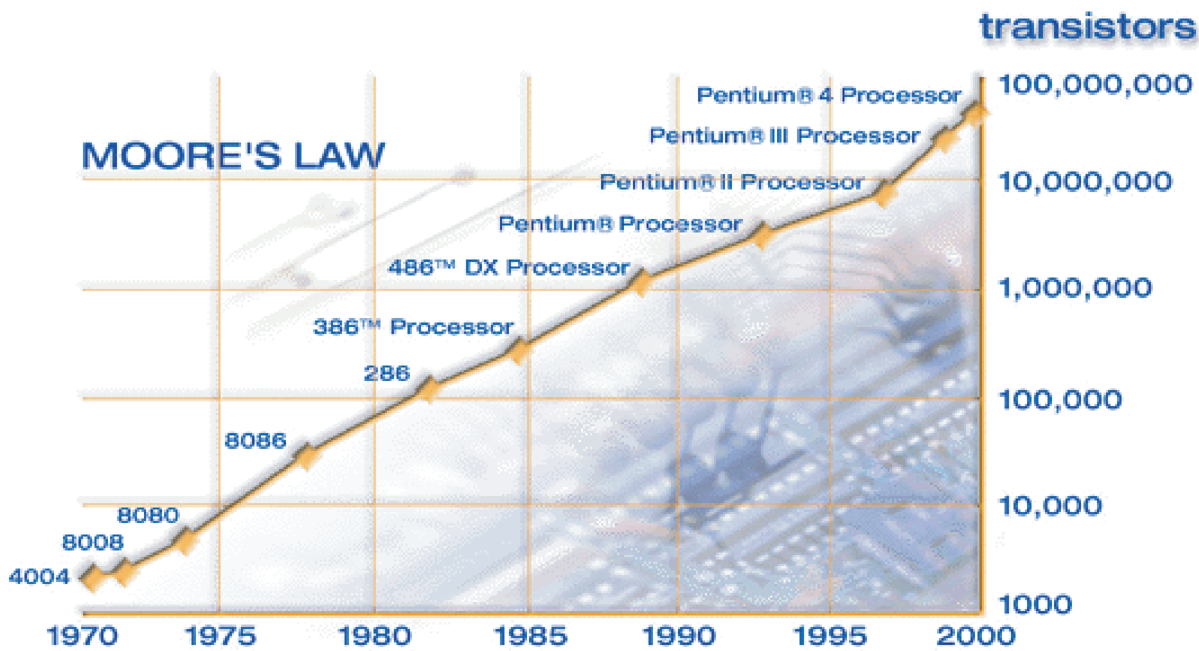
- The 1949 computation of $\pi$ to 2,037 places suggested by von Neumann, took 70 hours

- It would have taken roughly 100,000 ENIACs to store the Smithsonian's picture!

$\otimes$ Now after 40 years of Moore's law . . .

> "Moore's Law" is now taken to be the assertion that semiconductor technology approximately doubles in capacity and performance roughly every 18 to 24 months

# ... To Moore's Law



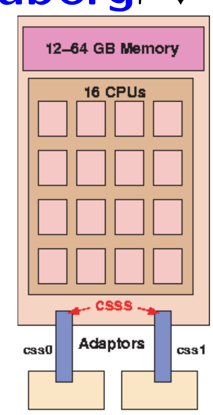

*The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. ... Over the longer term, the rate of increase is a bit more uncertain, although there is no reason to believe it will not remain nearly constant for at least 10 years.** (Gordon Moore, Intel co-founder, 1965)

*'Expect at least another decade.' (Moore et al)

- An astounding record of sustained exponential progress without peer in history of technology

- Math tools are now being implemented on parallel platforms, providing *much* greater power to the research mathematician

↶**NERSC's 6656cpu Seaborg**↷




727-fold speed-up of *quadrature* on the 1K G5's at **Virginia Tech** reduces **3hrs** to **15secs**

- Amassing huge amounts of processing power will not solve many mathematical problems. There are few math 'Grand-challenge problems' —more value in very rapid 'Aha's.

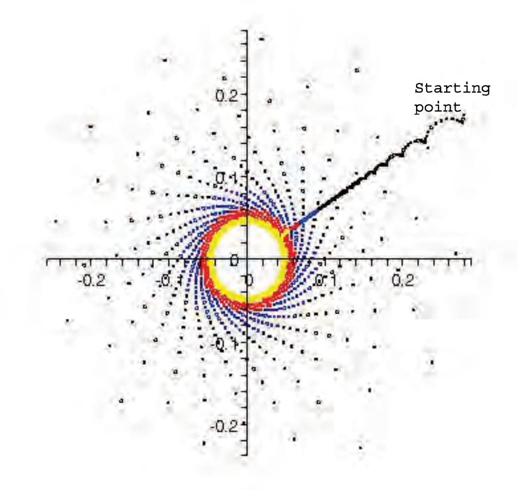
## VISUAL DYNAMICS

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

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

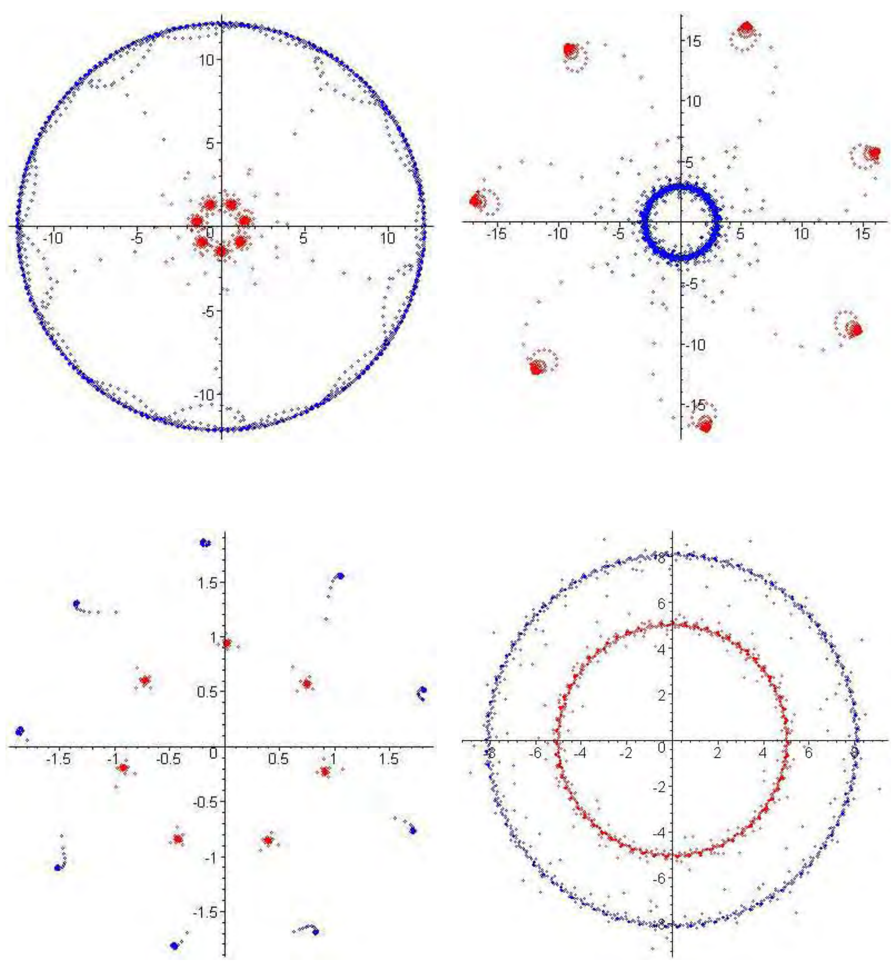
where $\omega_n = a^2, b^2$ for $n$ even, odd respectively.
✓ Think of this as a **black box**.

▷ Numerically all one *sees* is $t_n \to 0$ 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. We now predict and validate:



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

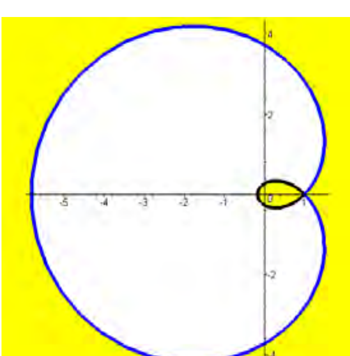
# RAMANUJAN'S FRACTION

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

$$\mathcal{R}_\eta(a,b) = \cfrac{a}{\eta + \cfrac{b^2}{\eta + \cfrac{4a^2}{\eta + \cfrac{9b^2}{\eta + \ddots}}}} \tag{1.1}$$

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

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



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

## HADAMARD and GAUSS

> 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.

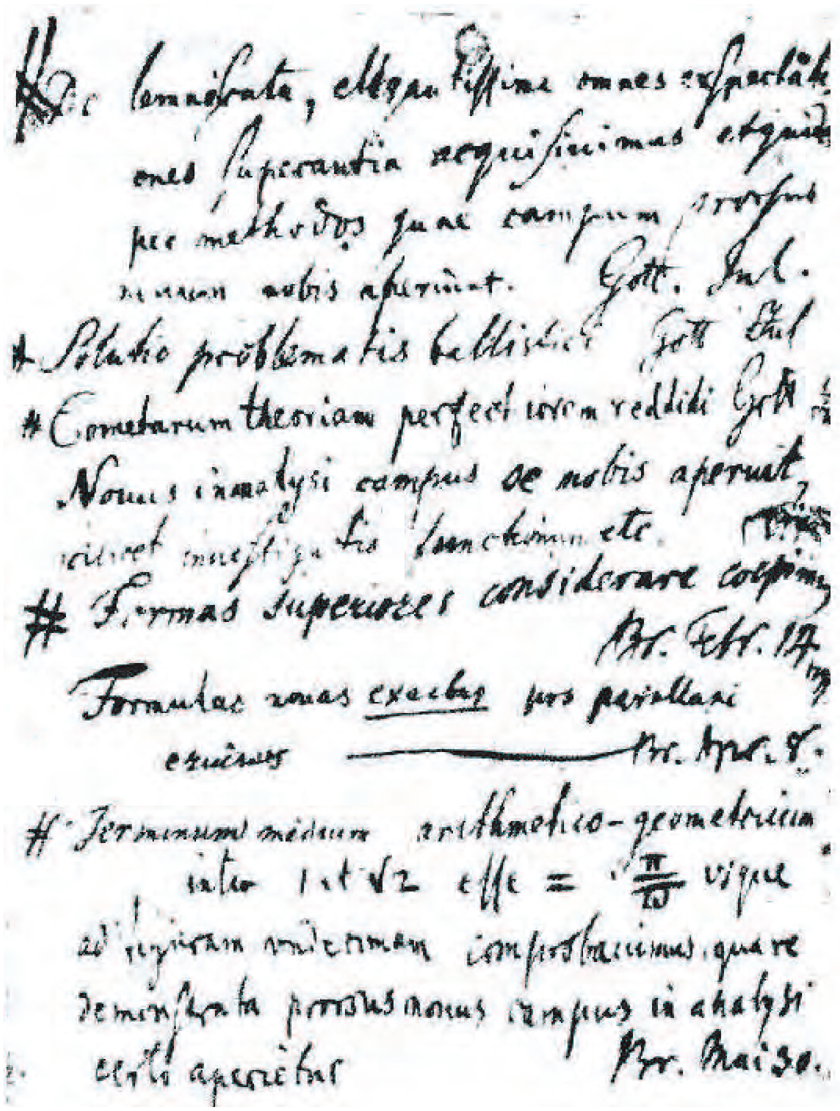
PAVCA SED MATVRA

MathResources Inc.

**Pauca sed Matura**

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.**

*Likewise the quote!



**Novus in analysi campus se nobis aperuit**

An excited young Gauss writes: "*A new field of analysis has revealed itself to us, evidently in the study of functions etc.*" (October 1798)

# 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. As does the status of the classification of Finite Simple Groups.

- Formal Proof theory has received an unexpected boost: automated proofs *may* now exist of: Four Color Theorem, Prime Number Theorem.

# 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. TURNLEY/S. SHERBELL/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[1,2]. 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[3]. 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.

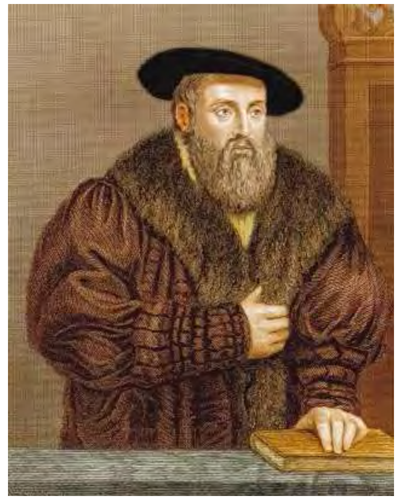
It was not enough for the referees to rerun Hales’s code — they had to check whether the programs did the job that they were supposed to do. Inspecting all of the code and its inputs and outputs, which together take up three gigabytes of memory space, would have been impossible. So the referees limited themselves to consistency checks, a reconstruction of the thought processes behind each step of the proof, and then a 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*[4]. 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."

S. TERRY/SPL



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

UNIV. PITTSBURGH CIDDE

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

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[5]. 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.**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Flyspeck
**www.math.pitt.edu/~thales/flyspeck/index.html**

# What in the Name of Euclid Is Going On Here?

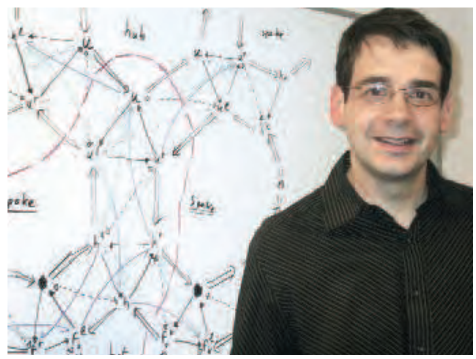
**Computer assistants may help mathematicians dot the i's and cross the t's of proofs so complex that they defy human comprehension**

In 1998, a young University of Michigan mathematician named Thomas Hales solved a nearly 4-century-old problem called the Kepler conjecture. The task was to prove that the standard grocery-store arrangement of oranges is, in fact, the densest way to pack spheres together. The editor of *Annals of Mathematics*, one of the most prestigious journals in mathematics, invited him to submit his proof to *Annals*. Neither of them was prepared for what happened next.

Over a period of 4 years, a team of 12 referees wrestled with the lengthy paper and eventually raised a white flag. They informed the editor that they were only "99 percent" certain that it was correct. In particular, they could not vouch for the validity of the lengthy computer calculations that were essential to Hales's proof. The editor took the unprecedented step of publishing the article with a disclaimer that it could not be absolutely verified (*Science*, 7 March 2003, p. 1513).

It is a scenario that has repeated itself, with variations, several times in recent years: A high-profile problem is solved with an extraordinarily long and difficult megaproof, sometimes relying heavily on computer calculation and often leaving a miasma of doubt behind it. In 1976, the Four Color Theorem started the trend, with a proof based on computer calculations so lengthy that no human could hope to follow them. The classification of finite simple groups, a 10,000-page multiauthor project, was completed (sort of) in 1980 but had to be recompleted last year. "We've arrived at a strange place in mathematics," says David Goldschmidt of the Institute for Defense Analyses in Alexandria, Virginia, one of the collaborators on the finite simple group proof. "When is a proof really a proof? There's no absolute standard." Goldschmidt thinks the traditional criterion—review by a referee (or team of them)—breaks down when a paper reaches hundreds or thousands of pages.

The computer—which at first sight seems to be part of the problem—may also be the solution. In the past few months, software packages called "proof assistants," which go through every step of a carefully written argument and check that it follows from the axioms of mathematics, have served notice that they are no longer toys. Last fall, Jeremy Avigad, a professor of philosophy at Carnegie Mellon University, used a computer assistant called Isabelle to verify the Prime Number Theorem, which (roughly speaking) describes the probability that a randomly chosen number in any interval is prime. And in December, Georges Gonthier, a computer scientist at Microsoft Research Cambridge, announced a successful verification of the proof of the Four Color Theorem, using a proof assistant called Coq. "It's finally getting to the stage where you can do serious things with these programs," says Avigad.



**Mapping the way.** Georges Gonthier's computer verified billions of calculations on "hypermaps" like the one shown.

Even Hales is getting into the action. Over the past 2 years, he has taught himself to use an assistant called HOL Light. In January, he became the first person to complete a computer verification of the Jordan Curve Theorem, first published in 1905, which says that any closed curve drawn in the plane without crossing itself separates the plane into two pieces.

For Hales, the motivation is obvious: He hopes, eventually, to vindicate his proof of the Kepler conjecture. In fact, three graduate students in Europe (not Hales's own) are already at work on separate parts of this project, two using Isabelle and one using Coq. Hales expects them to finish in about 7 years.

But Hales thinks that computer verifiers have implications far beyond the Kepler conjecture. "Suppose you could check a page a day," he says. "At that point it would make sense to devote the resources to put 100,000 pages of mathematics into one of these systems. Then the mathematical landscape is entirely changed." At present, computer assistants still take a lot of time to puzzle through some facts that even an advanced undergraduate would know or be able to figure out. With a large enough knowledge base, that particular time sink could be eliminated, and the programs might enable mathematicians to work more efficiently. "My own experience is that you spend a long time going over and going over a proof, making sure you haven't missed anything," says Carlos Simpson, an algebraic geometer and computer scientist at the University of Nice in France. "With the computer, once it's proved, it's proved. You only have to do it once, and the computer makes sure you get all the details."

In fact, computer proof assistants could change the whole concept of proof. Ever since Euclid, mathematical proofs have served a dual purpose: certifying *that* a statement is true, and explaining *why* it is

## Have a Coq and a Smile

Why would hundreds of computer scientists devote more than 30 years to developing mathematical proof assistants that most mathematicians don't even want? The answer is that they are chasing an even more elusive grail: self-checking computer code.

In a sense, the statement "this program (or chip, or operating system) performs task *x* correctly" is a mathematical theorem, and programmers would love to have that kind of certainty. "Currently, people who have experience with programming 'know' that serious programs without bugs are impossible," Freek Wiedijk and Henk Barendregt, computer scientists at the University of Nijmegen in the Netherlands, wrote in 2003. "However, we think that eventually the technology of computer mathematics … will change this perception."

Already, leading chip manufacturers use computer proof assistants to make sure their circuit designs are correct. Advanced Micro Devices uses a proof checker called ACL2, and Intel uses HOL Light. "When the division algorithm turned out to be wrong on the Pentium chip, that was a real wake-up call to Intel," says John Harrison, who designed HOL Light and was subsequently hired as a senior software engineer by Intel. **–D.M.**

CREDIT: COURTESY OF GEORGES GONTHIER

## MORE of OUR 'METHODOLOGY'

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

2. *Pattern Recognition of Real Numbers* (The Inverse Symbolic Calculator* and 'identify' or 'Recognize')

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

3. *Pattern Recognition of Sequences* (Salvy & Zimmermann's 'gfun', Sloane & Plouffe's *Encyclopedia*).

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

   ✓ "Exclusion bounds" are especially useful

   ✓ Great test bed for "Experimental Math"

5. 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.

## Another Truth

$$\frac{24}{7\sqrt{7}} \int_{\pi/3}^{\pi/2} \log \left| \frac{\tan t + \sqrt{7}}{\tan t - \sqrt{7}} \right| dt \stackrel{?}{=} L_{-7}(2) \qquad (5)$$

where

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

"Identity" (5) has been verified to 10,000 places. I have *no idea* of how to prove it.

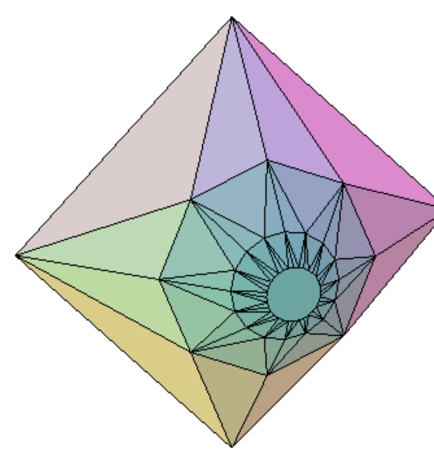
- A 64-CPU run (7250 secs) and a 256-CPU run (1855 secs) on the *Virginia Tech G5 cluster* agreed precisely—a *week in an hour*—the largest numerical quadrature calculation ever done?

- Equation (5) arises from the *volume of an ideal tetrahedron in hyperbolic space*.

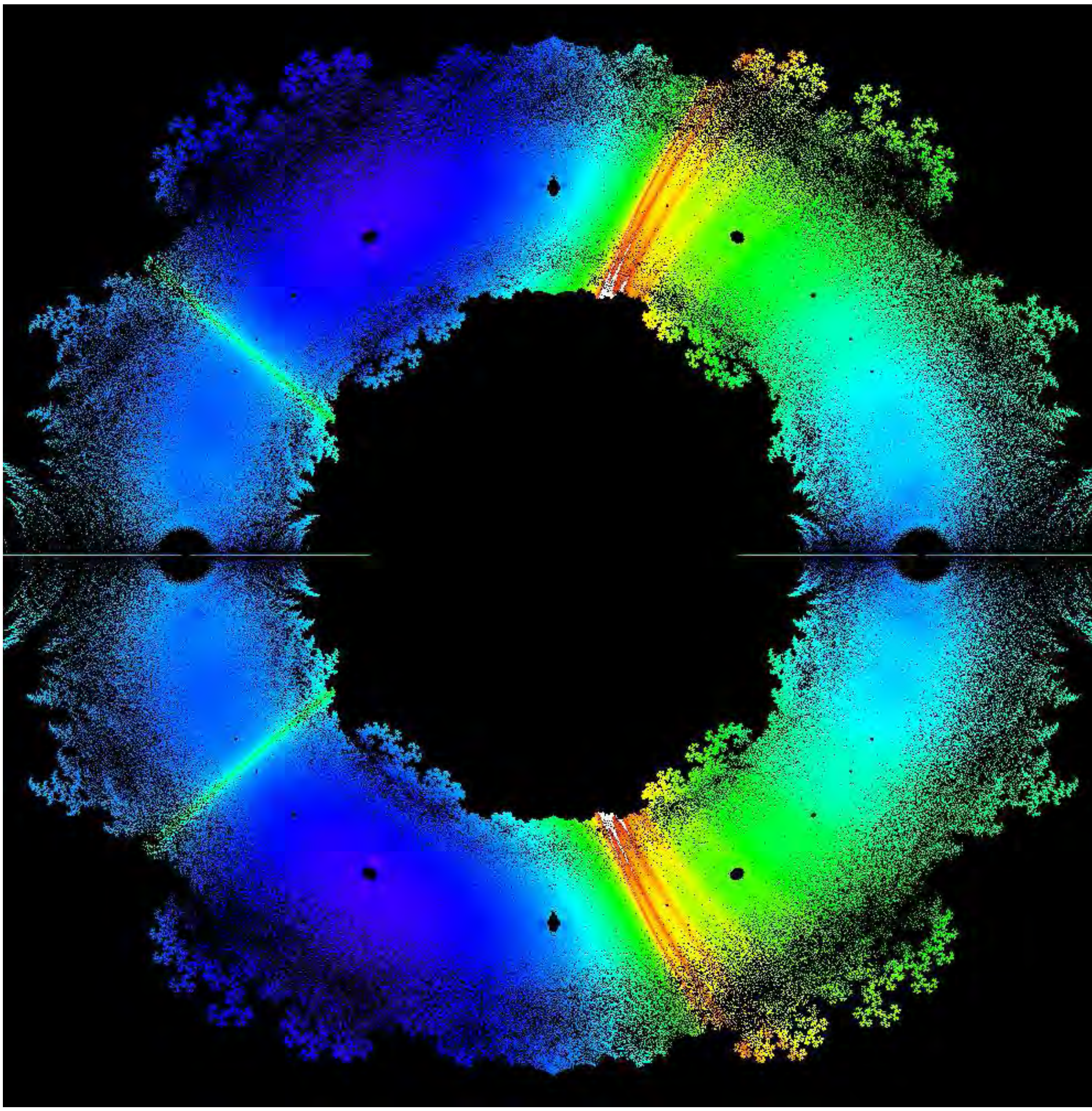
⊛ For algebraic topology reasons, it is known that the ratio of the left hand to the right hand side of (5) is rational.

# JOHN 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.*



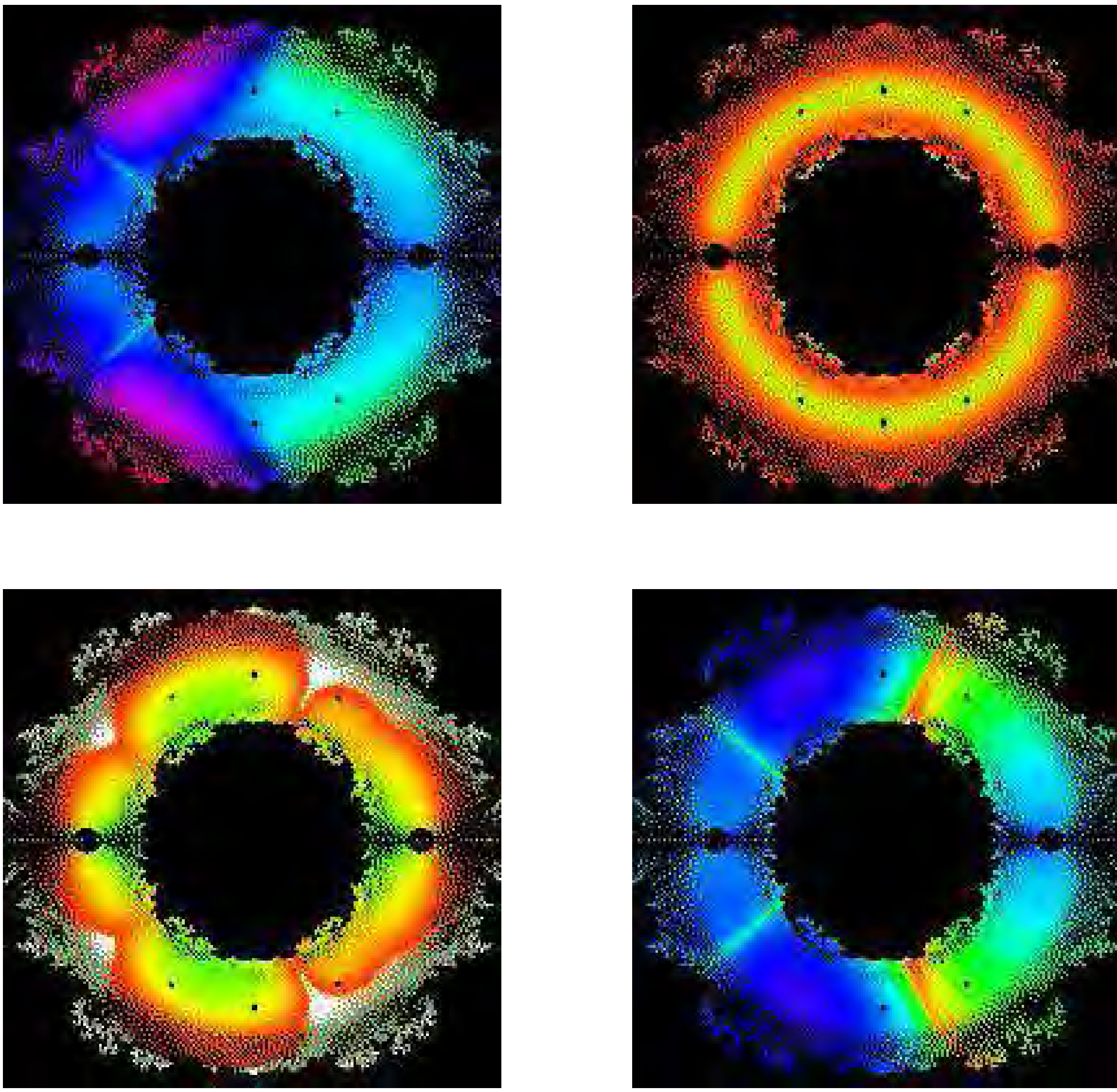
# ZEROES of $0-1$ POLYNOMIALS



**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)

# SEEING PATTERNS in PARTITIONS

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

$$1 + \sum_{n \geq 1} p(n) q^n = \frac{1}{\prod_{n \geq 1}(1 - q^n)}. \qquad (6)$$

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 (6) 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 1900 table for $p(n)$ to intuit remarkable deep congruences like

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

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

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

$$\begin{aligned} 1 \;+\;& q + 2\,q^2 + 3\,q^3 + \underline{5}\,q^{\mathbf{4}} + \overline{7}\,q^{\mathbf{5}} + 11\,q^6 + 15\,q^7 \\ +\;& 22\,q^8 + \underline{30}\,q^{\mathbf{9}} + 42\,q^{10} + 56\,q^{11} + \overline{77}\,q^{\mathbf{12}} \\ +\;& 101\,q^{13} + \underline{135}\,q^{\mathbf{14}} + 176\,q^{15} + 231\,q^{16} \\ +\;& 297\,q^{17} + 385\,q^{18} + \boxed{490}\,q^{\mathbf{19}} + 627\,q^{20} \\ +\;& 792\,q^{21} + 1002\,q^{22} + 1255\,q^{23} + \underline{1575}\,q^{\mathbf{24}} \\ +\;& \cdots + 3972999029388\,q^{200} + \cdots \end{aligned} \qquad (7)$$

- Cases $5n+4$ and $7n+5$ are flagged in (7)
  - leading to the *crank* (Dyson, Andrews, Garvan, Ono, and very recently Mahlburg)
  - connections with modular forms much facilitated by symbolic computation

- 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 (6).

- By **2000**, *Maple* produced $p(200)$ in seconds simply as the 200'th term of the Taylor series (ignoring '*combinat[numpart]*')

- 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 (6), 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 and learn about the *pentagonal numbers* occurring above in Neil *Sloanes*' exemplary on-line

  '*Encyclopedia of Integer Sequences*':

  `www.research.att.com/personal/njas/sequences/eisonline.html`

⊛ Such *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 often 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

**BERLINSKI**

*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.*

· · · and · · ·

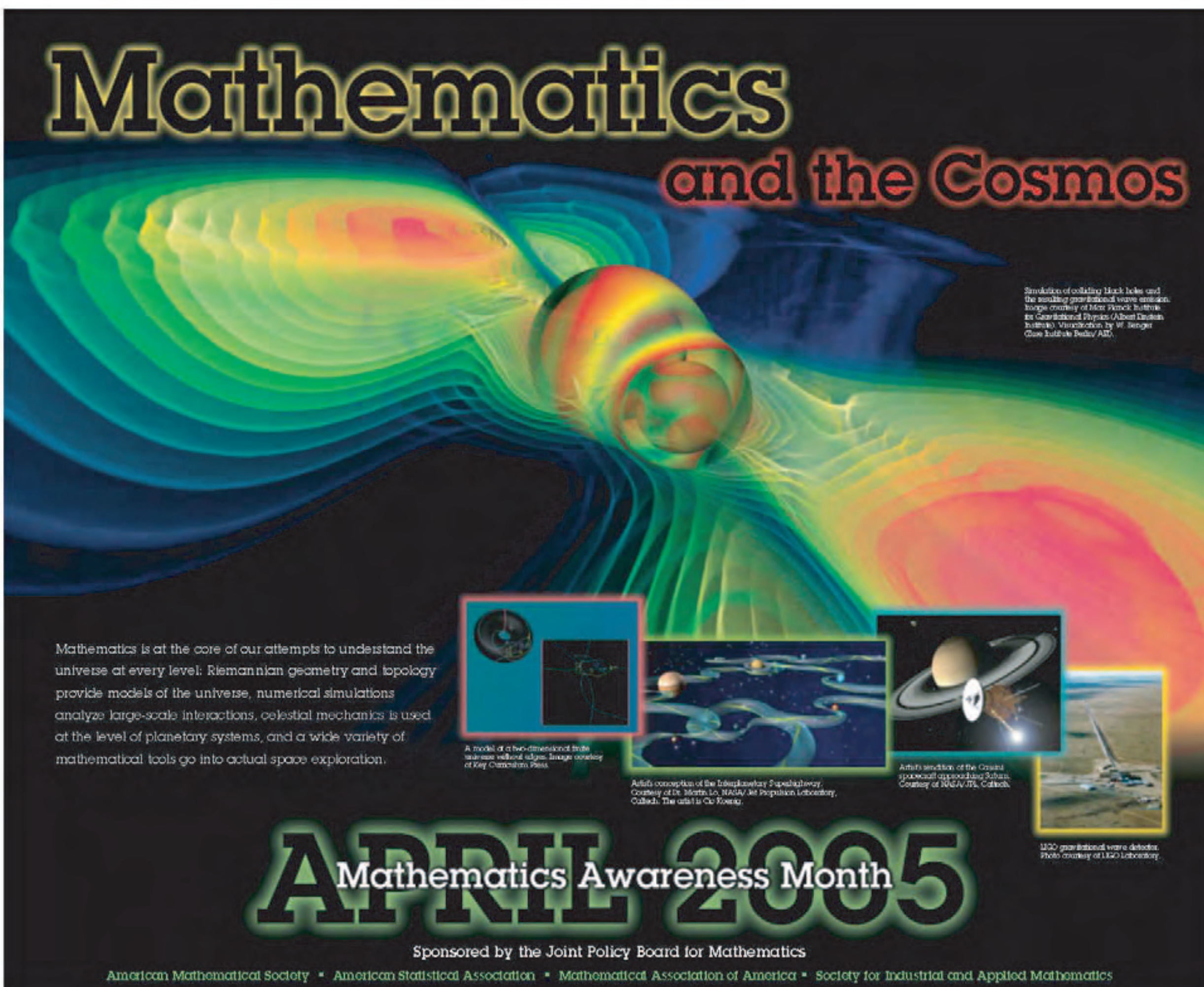
The computer has in turn changed the very nature of mathematical experience, *suggesting for the first time that mathematics, like physics, may yet become an empirical discipline, a place where things are discovered because they are seen.* (David Berlinski, 1997)*

- 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 again delightfully blurred.

- An early exciting example is provided by gravitational boosting:

*In "Ground Zero", a Review of *The Pleasures of Counting*, by T. W. Koerner.

- *Interactive graphics* will become an integral part of mathematics: gravitational boosting, gravity waves, Lagrange points, many-body problems . . .



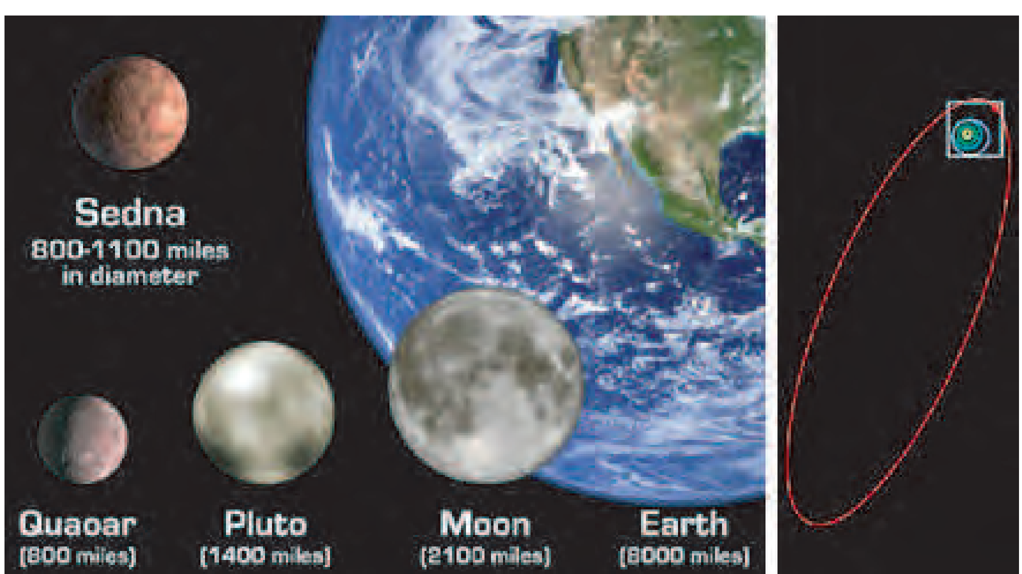

**1905** Special relativity, Brownian motion, Photoelectricity

## Gravitational Boosting

"The Voyager Neptune Planetary Guide" (JPL Publication 89–24) has an excellent description of Michael Minovitch's 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

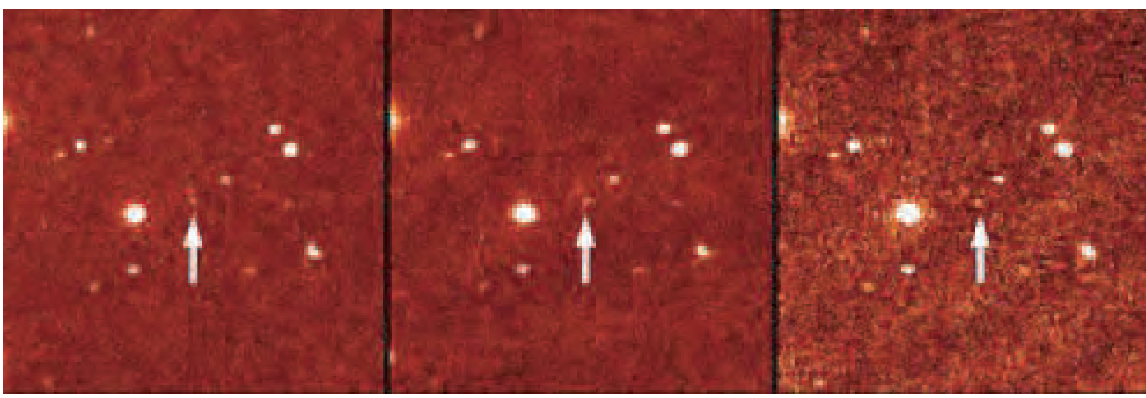
*"Any sufficiently advanced technology is indistinguishable from magic."*




**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).

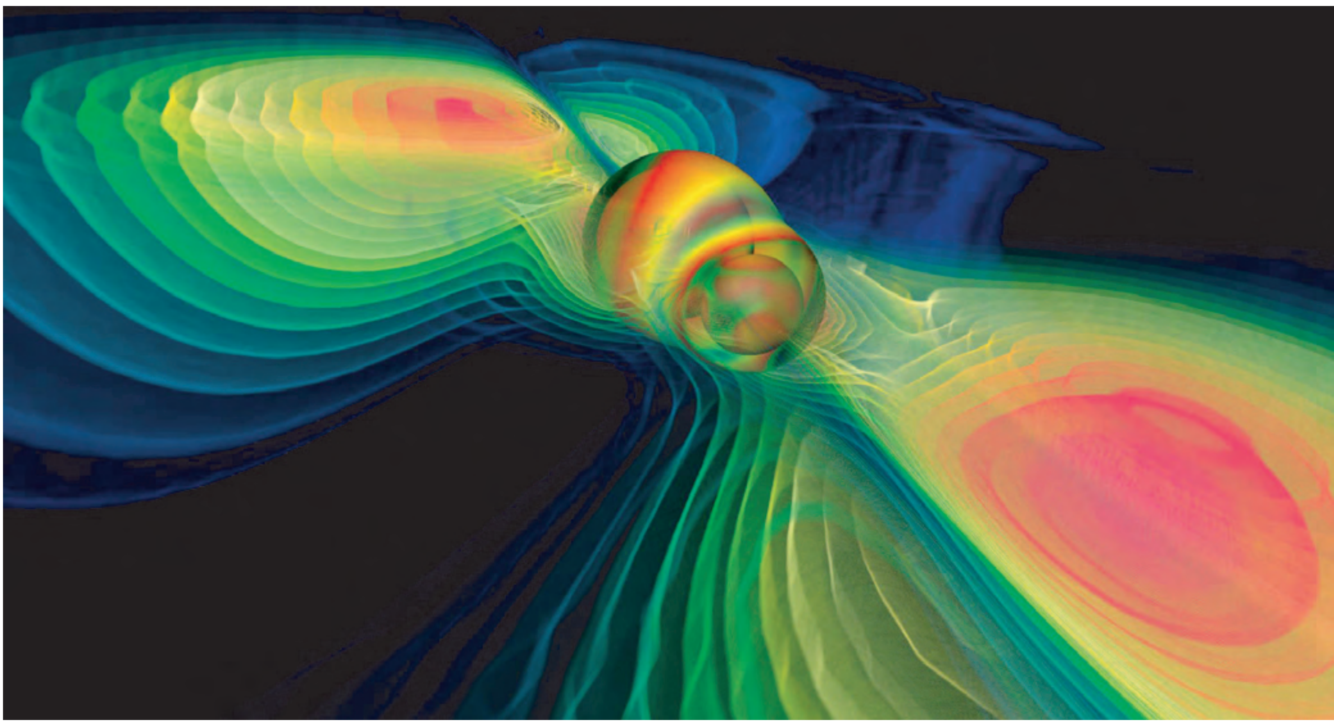
## LIGO: Math and the Cosmos

**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* (`www.westgrid.ca`)

# SOME CONCLUSIONS

> *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.* (Thomas Kuhn)

- 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."* (Einstein)

## 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, 1900)

- 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 tangible **Riemann surface for Lambert-**$W$

*A like article is in the 2004 *Mathematical Intelligencer*.

## FINAL COMMENTS

★ 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`

# HOW NOT TO EXPERIMENT


**Pooh Math**

**'Guess and Check'**
while
**Aiming Too High**

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*All references are at D-drive and `www.cecm.sfu.ca/preprints`.

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▶ The web site is at **www.expmathbook.info**

# APPENDIX I. ANOTHER CASE STUDY

## 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 $nth$ moment of a *Poisson distribution* with parameter $t$. Let $\mathbf{c_n(t) = m_n(t)/n!}$ . 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

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

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

$$1,1,2,5,15,52,203,877,4140\ldots.$$

- These are the *Bell numbers* as was discovered by consulting *Sloane's Encyclopedia*.

  `www.research.att.com/personal/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

$$\sum_{n\geq 0} c_n u^n = \exp\left(t(e^u - 1)\right). \tag{8}$$

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

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

**Theorem 1** *If a sequence* $1, b_1, b_2, \cdots$ *is non-negative and log-concave then so is the sequence* $1, c_1, c_2, \cdots$ *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 (8) above, we apply this to the sequence $\mathbf{b_j = t/(j-1)!}$ 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:

**(??)** $\Rightarrow$ Computer Algebra System $\Rightarrow$ Interface

$\Rightarrow$ Search Engine $\Rightarrow$ Digital Library

$\Rightarrow$ Hard New Paper $\Rightarrow$ **Answer**

★ Now if only we could automate this!

## APPENDIX II: INTEGER RELATIONS

## The USES of LLL and PSLQ

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

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

**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

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

- 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 `PSLQ` on

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

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

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

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

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

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

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

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

  [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

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

▶ 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. ZAGIER'S CONJECTURE

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

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

Thus

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

is the classical *polylogarithm*, while

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

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

These polylogarithms

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

are *determined uniquely* by the *differential equations*

$$\frac{d}{dx} L(\mathbf{n_r}, \ldots, n_1; x) = \frac{1}{x} L(\mathbf{n_r - 1}, \ldots, n_2, n_1; x)$$

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

$$\frac{d}{dx} L(\mathbf{n_r}, \ldots, n_2, n_1; x) = \frac{1}{1-x} L(\mathbf{n_{r-1}}, \ldots, n_1; x)$$

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

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

for $r \geq 1$ and

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

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

Then every *periodic* polylogarithm leads to a function

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

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 $\mathbf{D_s F = t^s F}$ 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:

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

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

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

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

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

▶ Indeed

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

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

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

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

$$\sum_{n=0}^{\infty} L(\underbrace{3, 1, 3, 1, \ldots, 3, 1}_{n-fold}; x)\, t^{4n} = F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; x\right) \times F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; x\right). \tag{9}$$

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

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

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 3** *(***Zagier Conjecture***)*

$$\zeta(\underbrace{3,1,3,1,\ldots,3,1}_{n-fold})=\frac{2\,\pi^{4n}}{(4n+2)!} \tag{10}$$

**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 (9) produces

$$F\left(\frac{t(1+i)}{2}, \frac{-t(1+i)}{2}; 1; 1\right) F\left(\frac{t(1-i)}{2}, \frac{-t(1-i)}{2}; 1; 1\right)$$

$$= \frac{2}{\pi^2 t^2} \sin\left(\frac{1+i}{2}\pi t\right) \sin\left(\frac{1-i}{2}\pi t\right)$$

$$= \frac{\cosh \pi t - \cos \pi t}{\pi^2 t^2} = \sum_{n=0}^{\infty} \frac{2\pi^{4n} t^{4n}}{(4n+2)!}$$

on using the Taylor series of cos and cosh. Comparing coefficients in (9) ends the proof. **QED**

- ▶ What other deep Clausen-like hypergeometric factorizations lurk within?

- • If one suspects that (3) 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 $\zeta(2n)$.