



Dalhousie Distributed Research Institute and Virtual Environment

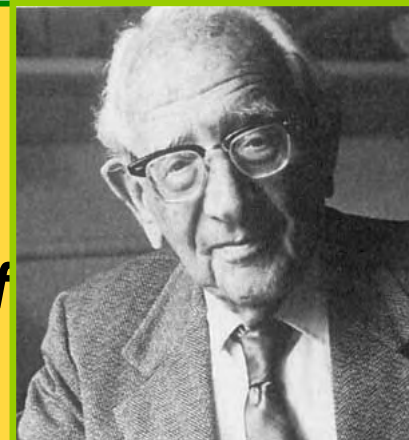
## What is HIGH PERFORMANCE MATHEMATICS?

Jonathan Borwein, FRSC [www.cs.dal.ca/~jborwein](http://www.cs.dal.ca/~jborwein)



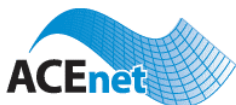
Canada Research Chair in Collaborative Technology

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



**George Polya**  
1887-1987

Atlantic Computational Excellence Network





Avatar: 1000.000  
Avatar: PC: camera  
Animation: OFF  
Position: (0, 0, 0)  
<http://www.cscn.edu>



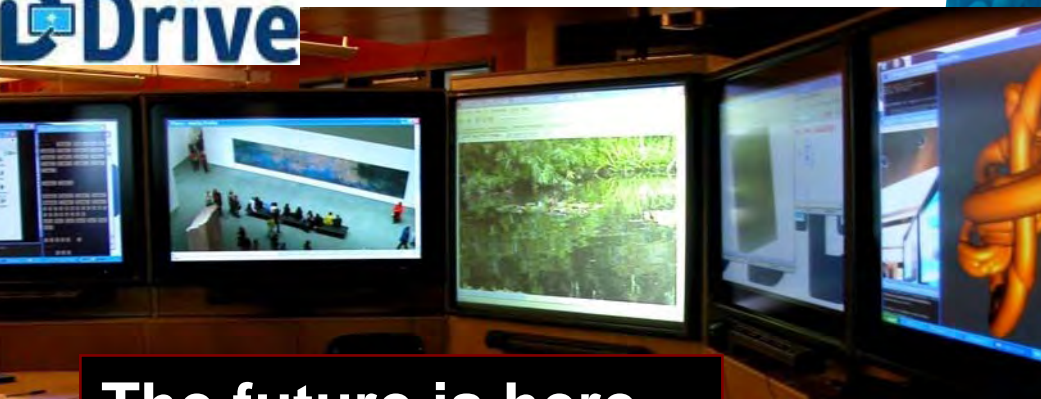
**2003: Me and my Avatar Designer now works for William Shatner ('Wild')**

# How-To Training Sessions



Brought to you using  
Access Grid  
technology

For more information contact Jana at 210-5489 or [jana@netera.ca](mailto:jana@netera.ca)



The future is here...

Remote Visualization via  
Access Grid

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

... just not uniformly



# What is HIGH PERFORMANCE MATHEMATICS?



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

**VOIP/SKYPE and a WEBCAM**

**MAPLE or MATLAB or ...**

**A REASONABLE LAPTOP**

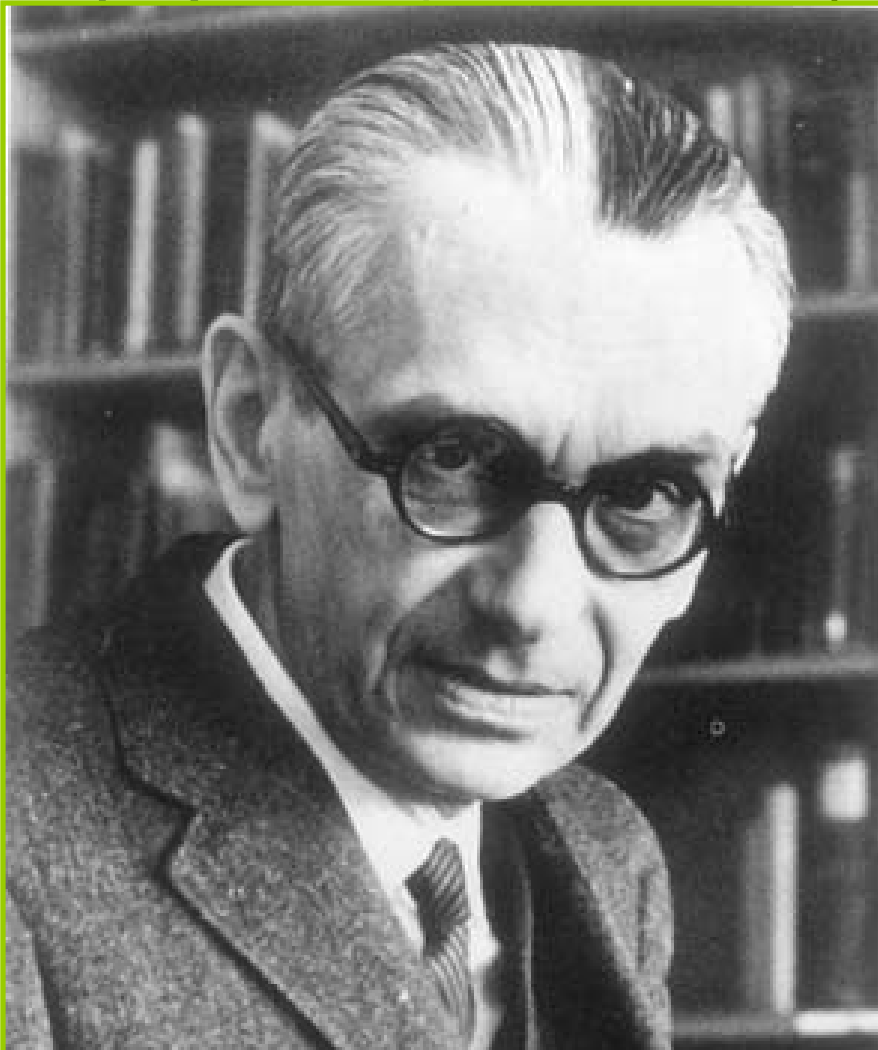
**A SPIRIT OF ADVENTURE**

**in almost all areas of mathematics**

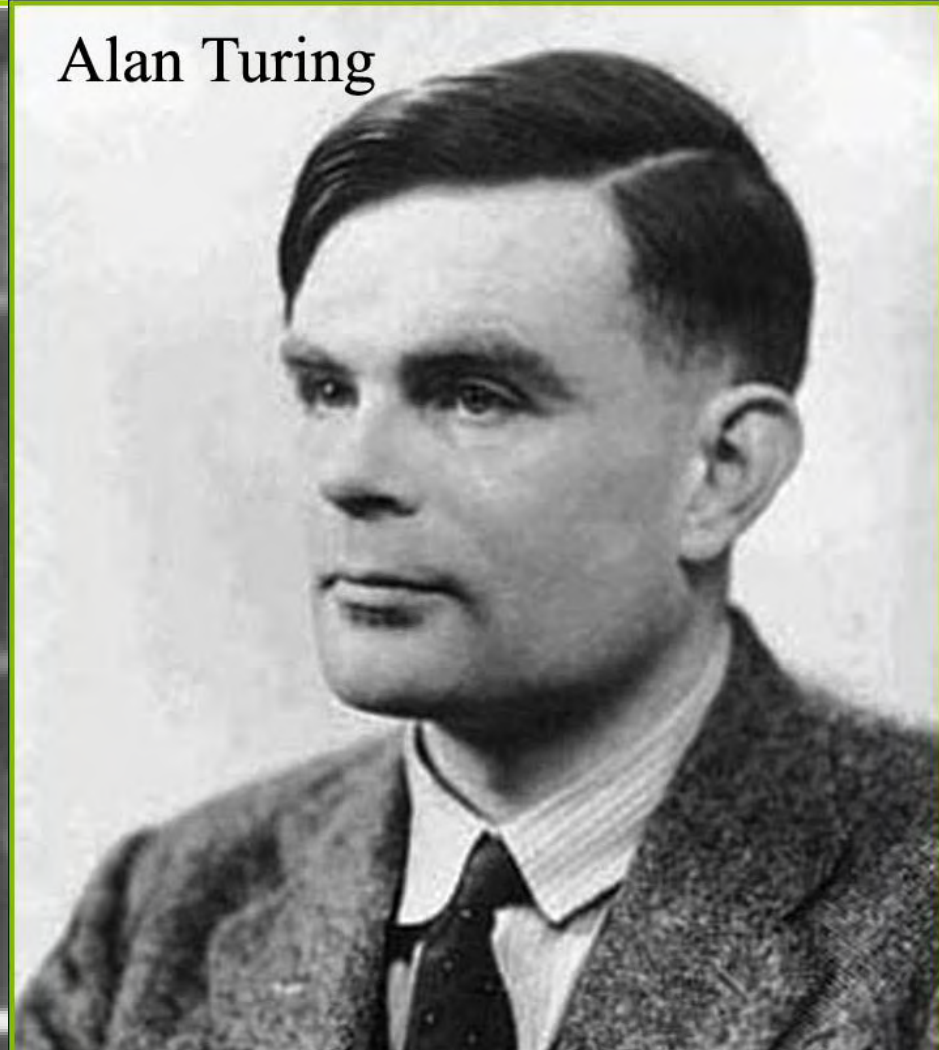
Drive

# ABSTRACT

*“If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics.”* (**Kurt Godel, 1951**)



Alan Turing



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

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

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

which is both numerically and symbolically quite challenging ....

and is answered at the end

# Outline. What is HIGH PERFORMANCE MATHEMATICS?

## 1a. Communication, Collaboration and Computation.

## 1b. Visual Data Mining in Mathematics.

- ✓ Fractals, Polynomials, Continued Fractions\*
- ✓ Pseudospectra and Code Optimization



## 2. High Precision Mathematics.

The talk ends  
when I do

## 3. Integer Relation Methods.

- ✓ Chaos, Zeta\* and the Riemann Hypothesis
- ✓ Hex-Pi and Normality



## 4. Inverse Symbolic Computation.

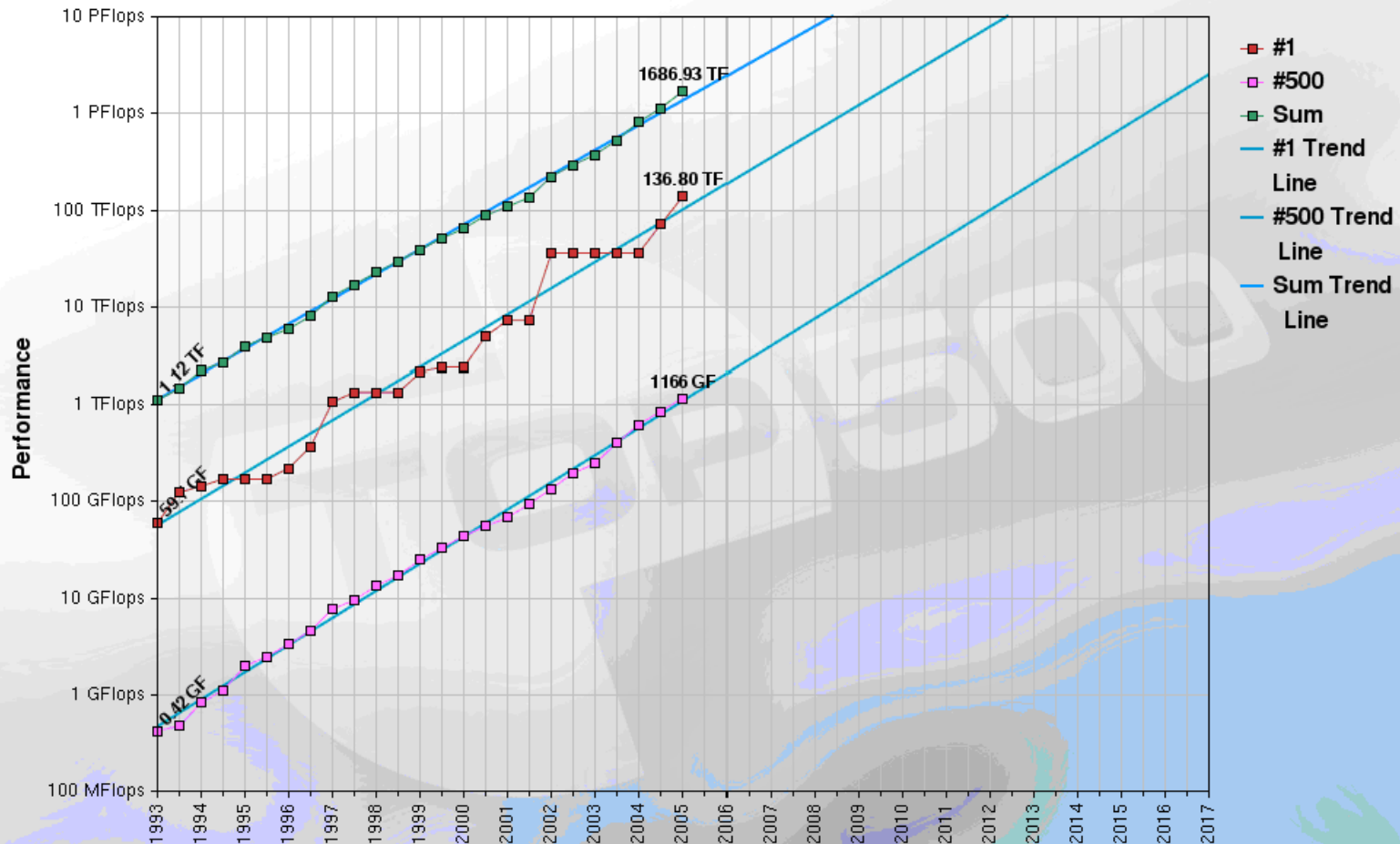
- ✓ A problem of Knuth\*,  $\pi/8$ , Extreme Quadrature

## 5. Demos and Conclusion.

# Moore's 1965 Law continues:



## Projected Performance Development

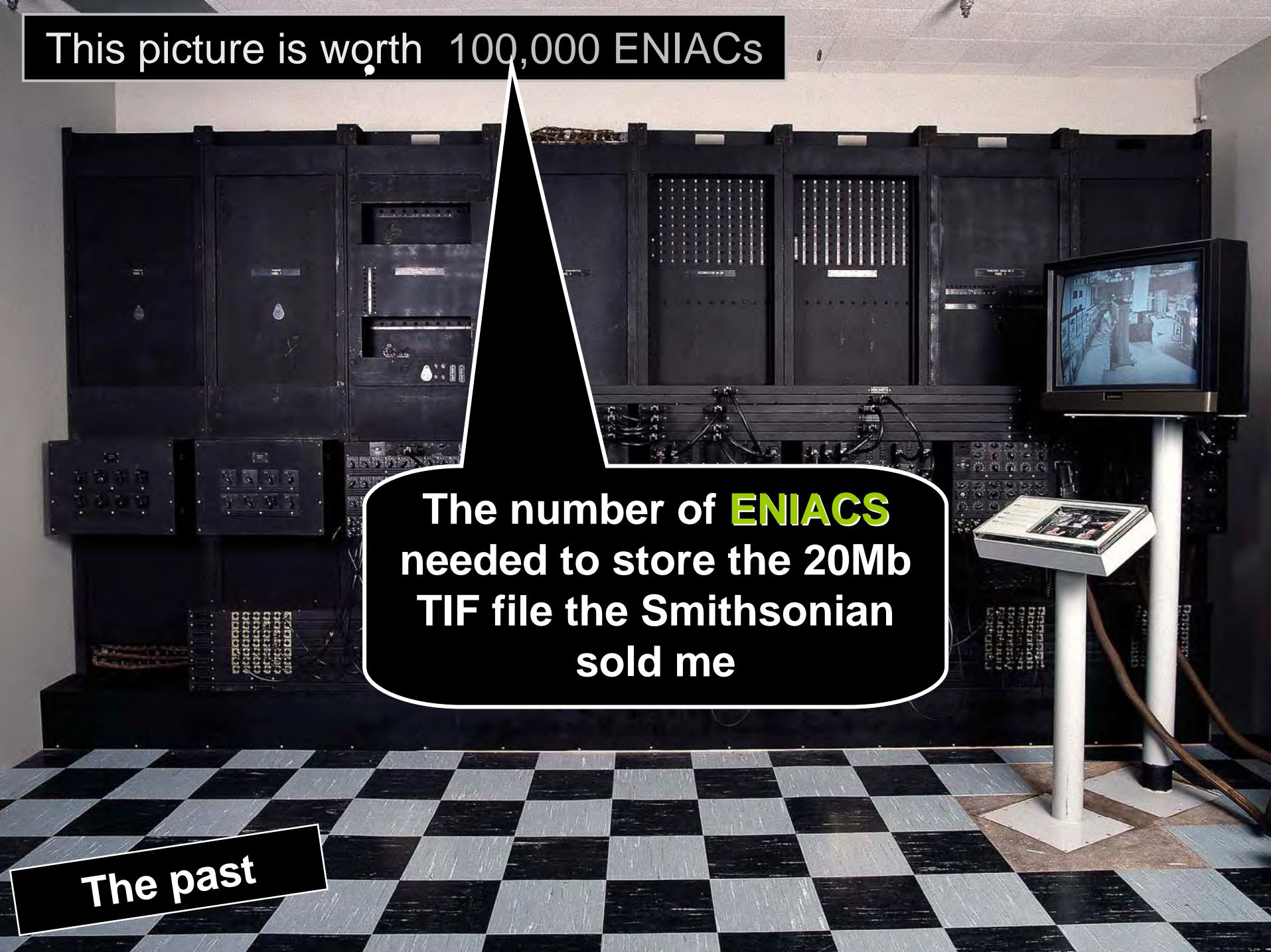




This picture is worth 100,000 ENIACs

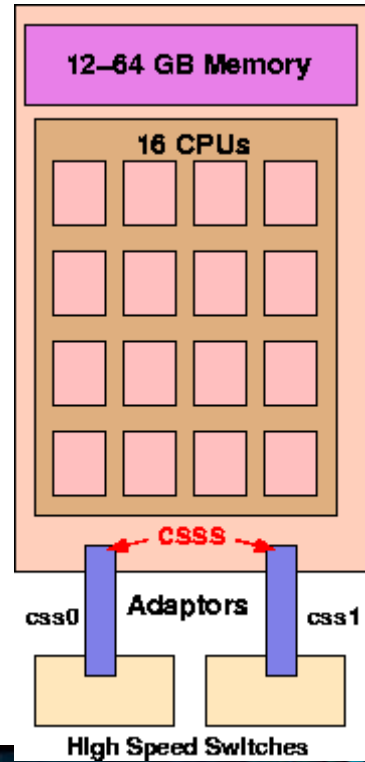
The number of **ENIACs** needed to store the 20Mb TIF file the Smithsonian sold me

The past



# NERSC's 6000 cpu Seaborg in 2004 (10Tflops/sec)

- we need new software paradigms for `bigga-scale' hardware



**The present**

**Mathematical Immersive Reality**  
in Vancouver

# IBM BlueGene/L system at LLNL

System  
(64 cabinets, 64x32x32)

## Supercomputer doubles own record

The Blue Gene/L supercomputer has broken its own record to achieve more than double the number of calculations it can do a second.

It reached 280.6 teraflops - that is 280.6 trillion calculations a second.



Blue Gene/L is the fastest computer in the world

2.8/5.6 GF/s  
4 MB

5.6/11.2 GF/s  
0.5 GB DDR

**The future**

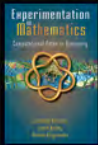
**2<sup>17</sup> cpu's**

**Oct 2005** It has now run Linpack benchmark at over **280 Tflop /sec**  
**(4 x Canadian-REN)**



*"It says it's sick of doing things like inventories and payrolls, and it wants to make some breakthroughs in astrophysics."*

# EXPERIMENTS IN MATHEMATICS



**Jonathan M. Borwein  
David H. Bailey  
Roland Girgensohn**

Produced with the assistance of Mason Macklem

*The reader who wants to get an introduction to this exciting approach to doing mathematics can do no better than this.*  
—Notices of the Royal Society

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

This *Experiments in Mathematics* CD contains the full text of both *Experiments in Mathematics: Plausible Reasoning in the 21st Century* and *Experimentation in Mathematics: Computational Paths to Discovery* in searchable form. The CD includes several "smart" enhancements:

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

These enhancements significantly improve the usability of these texts and the reader's experience with the material.

ISBN 1-5



9 781568 812830



A K Peters, Ltd.

Borwein  
Bailey  
Girgensohn



A K PETERS

## EXPERIMENTS IN MATHEMATICS

**Jonathan M. Borwein  
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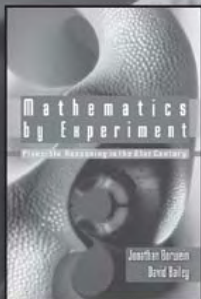
A K Peters, Ltd.

**Jonathan M. Borwein, David H. Bailey, Roland Girgensohn**

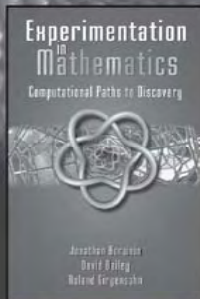
Produced with the assistance of Mason Macklem

"I do not think that I have had the good fortune to read two more entertaining and informative mathematics texts."

—*Gazette of the Australian Mathematical Society*



+



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## Experiments in Mathematics

Jonathan M. Borwein, David H. Bailey, Roland Girgensohn

In a short time since the first editions of *Mathematics by Experiment: Plausible Reasoning in the 21st Century* and *Experimentation in Mathematics: Computational Paths to Discovery*, we have seen a noticeable upsurge in interest in using computers to do real mathematics. The authors have updated and enhanced the book files and have now made them available in PDF form on CD-ROM. The CD includes several "smart" enhancements, including:

- Hyperlinks for all cross references (including theorems, figures, equations, etc.)
- Hyperlinks for all Internet URLs
- Hyperlinks for bibliographic references

The integrated search facility assists one with a search for particular mathematical formulations. These enhancements will significantly improve the usability of these files and the overall reading experience.

ROM

ISBN 1-56881-283-3

Call: 781.416.2888  
Email: [service@akpeters.com](mailto:service@akpeters.com)

[www.akpeters.com](http://www.akpeters.com)



## Experimental Mathematics in Action

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

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

Specific case studies include:

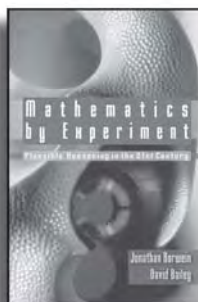
- analytic evaluation of integrals by means of symbolic and numeric computing techniques
- evaluation of Apery-like summations
- finding dependencies among high-dimension vectors (with applications to factoring large integers)
- inverse scattering (reconstruction of physical objects based on electromagnetic or acoustic scattering)
- investigation of continuous but nowhere differentiable functions.

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

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

### Mathematics by Experiment: Plausible Reasoning in the 21st Century

Jonathan Borwein, David Bailey



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

— *Notices of the AMS*

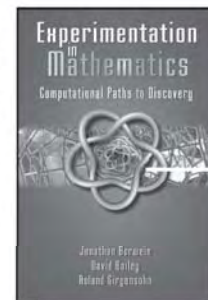
ISBN 1-56881-211-6; Hardcover; 298 pp.; \$45.00

### Experimentation in Mathematics: Computational Paths to Discovery

Jonathan Borwein, David Bailey, Roland Girgensohn

"These are such fun books to read! Actually, calling them books does not do them justice. They have the liveliness and feel of great Web sites, with their bite-size fascinating factoids and their many human- and math-interest stories and other gems. But do not be fooled by the lighthearted, immensely entertaining style. You are going to learn more math (experimental or otherwise) than you ever did from any two single volumes. Not only that, you will learn by osmosis how to become an experimental mathematician."

— *American Scientist*



ISBN 1-56881-136-5; Hardcover; 368 pp.; \$49.00

# Experimental Methodology

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

## MATH LAB

Computer experiments are transforming mathematics

BY ERICA KLARREICH

Science News  
2004

**M**any 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.

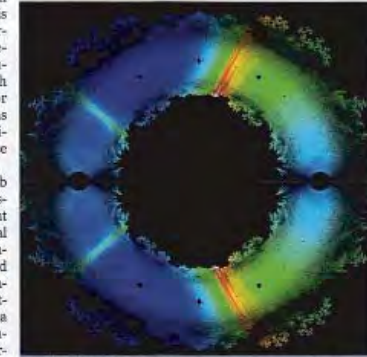
For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time."

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  $x$ .

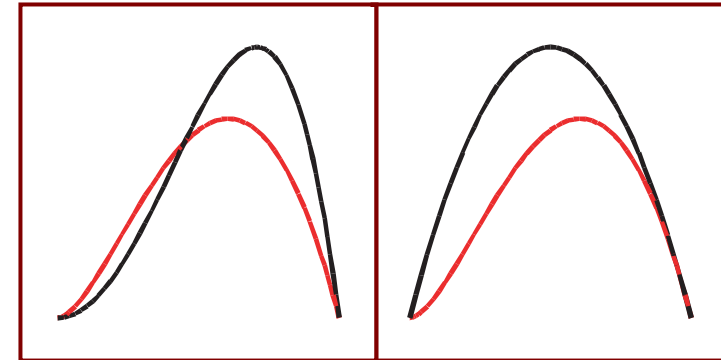
Gauss often discovered results experimentally long before he could prove them formally. Once, he complained, "I have the result, but I do not yet know how to get it."

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 calculation.



**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.



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

# 1 PARTIAL FRACTIONS and CONVEXITY

In a coupon collection thesis at SFU

- We consider a network *objective function*  $p_n$  given by

$$p_n(\vec{q}) = \sum_{\sigma \in S_n} \left( \prod_{i=1}^n \frac{q_{\sigma(i)}}{\sum_{j=i}^n q_{\sigma(j)}} \right) \left( \sum_{i=1}^n \frac{1}{\sum_{j=i}^n q_{\sigma(j)}} \right)$$

summed over *all*  $n!$  permutations; so a typical term is

$$\left( \prod_{i=1}^n \frac{q_i}{\sum_{j=i}^n q_j} \right) \left( \sum_{i=1}^n \frac{1}{\sum_{j=i}^n q_j} \right) .$$



**This looked pretty ugly**  
but Ian Affleck hoped  $p_n$  was convex !

◇ For  $n = 3$  this is

**6 TERMS LIKE**

$$q_1 q_2 q_3 \left( \frac{1}{q_1 + q_2 + q_3} \right) \left( \frac{1}{q_2 + q_3} \right) \left( \frac{1}{q_3} \right) \\ \times \left( \frac{1}{q_1 + q_2 + q_3} + \frac{1}{q_2 + q_3} + \frac{1}{q_3} \right) .$$

● We wish to show  $p_n$  is *convex* on the positive orthant. First we try to simplify the expression for  $p_n$ .

**COMPUTERS DO SOME THINGS  
BETTER THAN US**

- The *partial fraction decomposition* gives:

$$p_1(x) = \frac{1}{x},$$

$$p_2(x_1, x_2) = \frac{1}{x_1} + \frac{1}{x_2} - \frac{1}{x_1 + x_2},$$

$$p_3(x_1, x_2, x_3) = \frac{1}{x_1} + \frac{1}{x_2} + \frac{1}{x_3} - \frac{1}{x_1 + x_2} - \frac{1}{x_2 + x_3} - \frac{1}{x_1 + x_3} + \frac{1}{x_1 + x_2 + x_3}.$$

So we predict the 'same' for  $N = 4$  and

**CHECK SYMBOLICALLY**

**CONJECTURE.** For each  $N \in \mathbb{N}$

$$p_N(x_1, \dots, x_N) := \int_0^1 \left( 1 - \prod_{i=1}^N (1 - t^{x_i}) \right) \frac{dt}{t}$$

is convex, indeed 1/concave.

**Non-convex integrand**

- Check  $N < 5$  via large symbolic Hessian

**PROOF.** A year later, *joint expectations* gave:

$$p_N(x) = \int_{\mathbb{R}_+^n} e^{-(y_1 + \dots + y_n)} \max \left( \frac{y_1}{x_1}, \dots, \frac{y_n}{x_n} \right) dy$$

[See *SIAM Electronic Problems and Solutions*.]

**Convex integrand**

Also in ToVA -- find a direct proof?

# True, but why ?

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

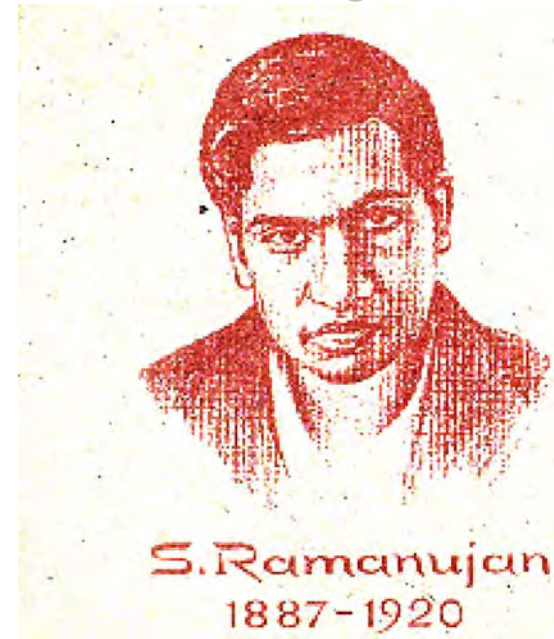
The candidates:

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

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

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

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



Here, in terms of factorials and rising factorials:

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

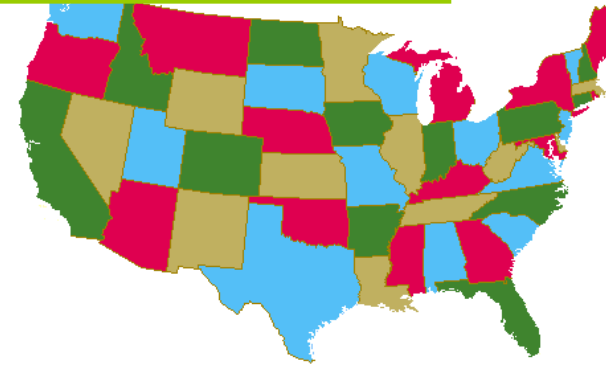
The 4<sup>th</sup> is **only** true

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

# Grand Challenges in Mathematics (CISE 2000)

are few and far between

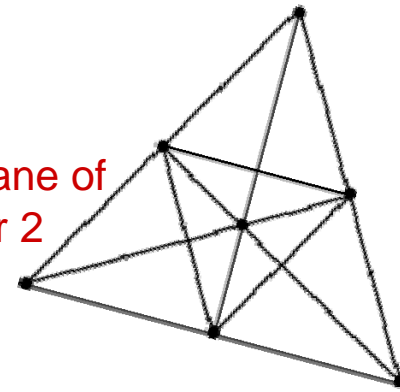
- **Four Colour Theorem** (1976,1997)
- **Kepler's problem** (Hales, 2004-12)



On an upcoming slide

- **Nonexistence of Projective Plane of Order 10**
  - $10^2+10+1$  lines and points on each other ( $n+1$  fold)
    - 2000 Cray hrs in 1990
    - next similar case: **18** needs  $10^{12}$  hours?
    - or a Quantum Computer

Fano plane of order 2



**Fermat's Last Theorem** (Wiles 1993, 1994)

- By contrast, any counterexample was too big to find (1985)

$$x^N + y^N = z^N, N > 2$$

has only trivial integer solutions



# Cultural Maps in Mathematics

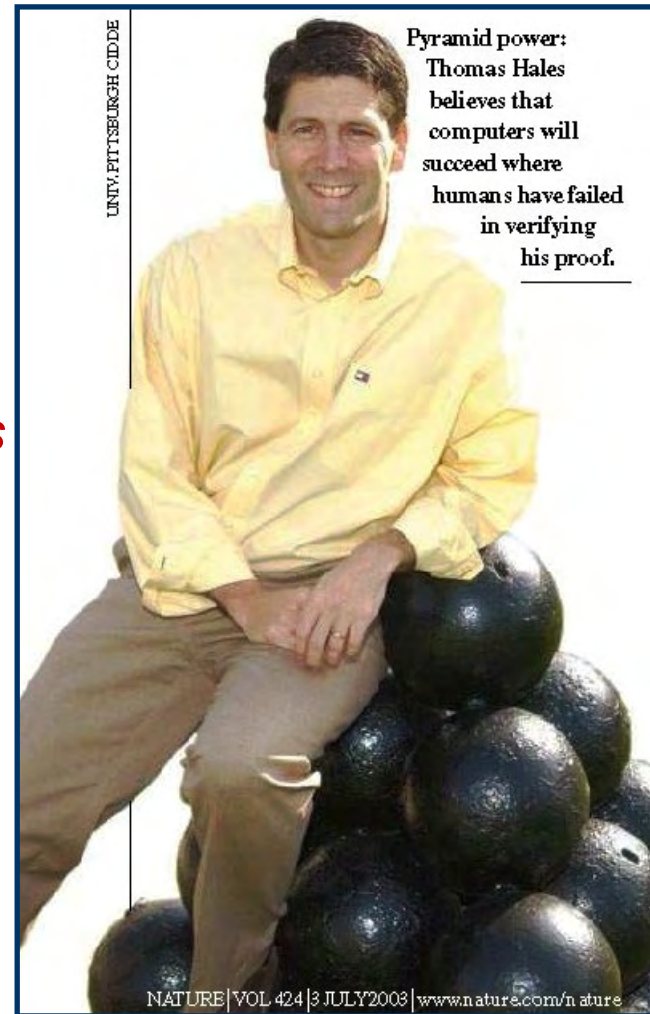
**“Mathematicians are a kind of Frenchmen:**

**whatever you say to them they translate into their own language, and right away it is something entirely different.”**

**(Johann Wolfgang von Goethe)**

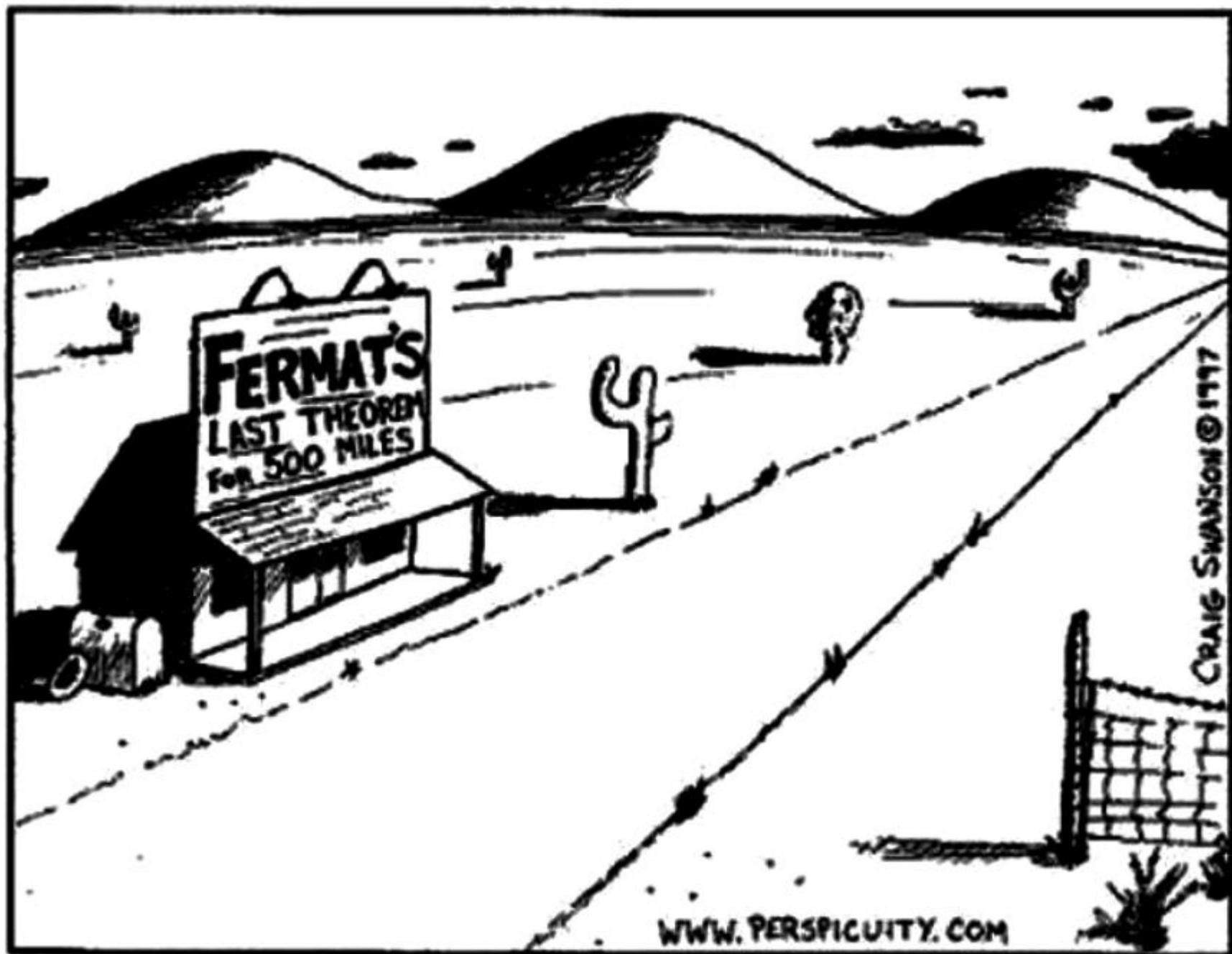
Maximen und Reflexionen, no. 1279

- **Kepler's conjecture** **the densest way to stack spheres is in a pyramid**
  - oldest problem in discrete geometry?
  - most interesting recent example of computer assisted proof
  - published in *Annals of Mathematics* with an “**only 99% checked**” disclaimer
  - Many varied reactions. *In Math, Computers Don't Lie. Or Do They?* (NYT, 6/4/04)
- **Famous earlier examples:** Four Color Theorem and Non-existence of a Projective Plane of Order 10.
  - the three raise quite distinct questions - both real and specious
  - as does status of classification of **Finite Simple Groups**



**Formal Proof theory** (code validation) has received an unexpected boost: automated proofs *may* now exist of the Four Color Theorem and Prime Number Theorem

- COQ: *When is a proof a proof?* Economist, April 2005



**FERMAT'S**  
**LAST THEOREM**  
**For 500 MILES**

CRAIG SWANSON © 1997

WWW.PERSPICUITY.COM





Dalhousie Distributed Research Institute and Virtual Environment

## East meets West: Collaboration goes National

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

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

Atlantic Computational Excellence Network



AARMS





Dalhousie Distributed Research Institute and Virtual Environment

## Coast to Coast Seminar Series



Lead partners:

**Dalhousie D-Drive** – Halifax  
Nova Scotia

**IRMACS** – Burnaby, British  
Columbia

Other Participants so far:

University of British Columbia, University of Alberta, University of Alberta University of Saskatchewan, Lethbridge University, Acadia University, St Francis Xavier University, University of Western Michigan, MathResources Inc, University of North Carolina

Tuesdays 3:30 – 4:30 pm Atlantic Time

<http://projects.cs.dal.ca/ddrive/>



Dalhousie Distributed Research Institute and Virtual Environment

# The Experience

Fully Interactive multi-way audio and visual

**Given good bandwidth audio is much harder**

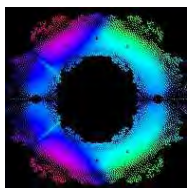
The closest thing to being in the same room



Shared Desktop for viewing presentations or sharing software



Dalhousie Distributed Research Institute and Virtual Environment



**Jonathan Borwein**, Dalhousie University  
**Mathematical Visualization**

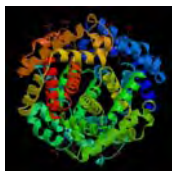
**High Quality Presentations**

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



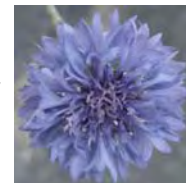
**Peter Borwein**, IRMACS  
**The Riemann Hypothesis**

**Jonathan Schaeffer**, University of Edmonton  
**Solving Checkers**



**Arvind Gupta**, MITACS  
**The Protein Folding Problem**

**Przemyslaw Prusinkiewicz**, University of Calgary  
**Computational Biology of Plants**

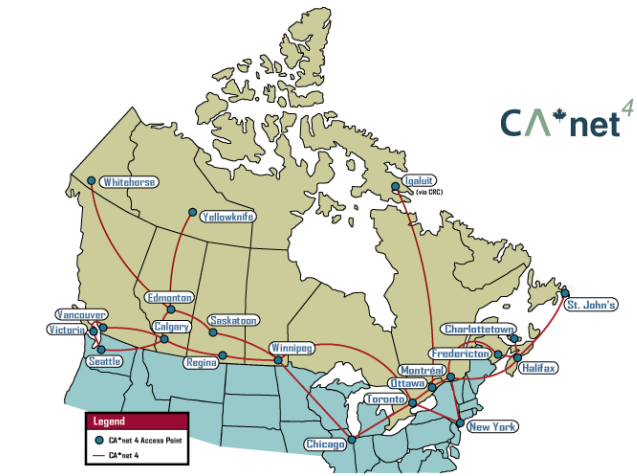


**Karl Dilcher**, Dalhousie University  
**Fermat Numbers, Wieferich and Wilson Primes**

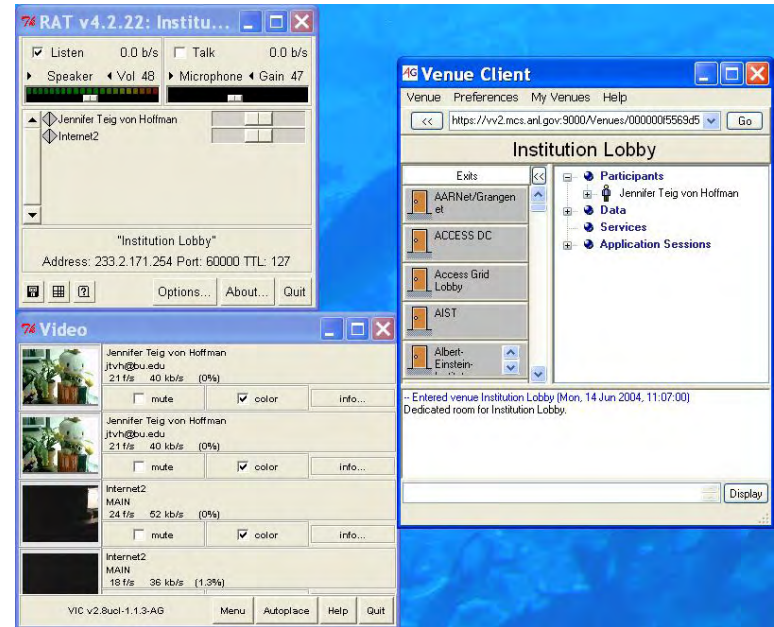
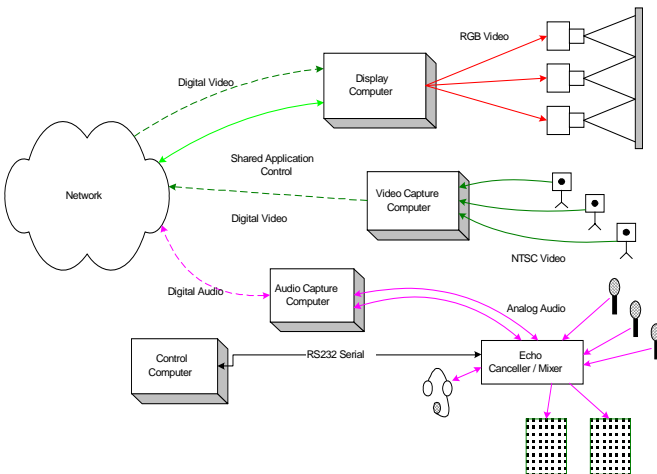


# Dalhousie Distributed Research Institute and Virtual Environment

## The Technology



High Bandwidth  
Connections  
(CA\*net)  
+  
PC Workstations  
+  
Audio/Video  
Equipment  
+  
Open Source  
Software





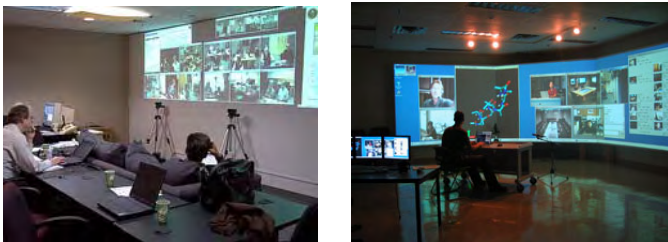
# Dalhousie Distributed Research Institute and Virtual Environment

**Personal Nodes**  
(1-4 people)



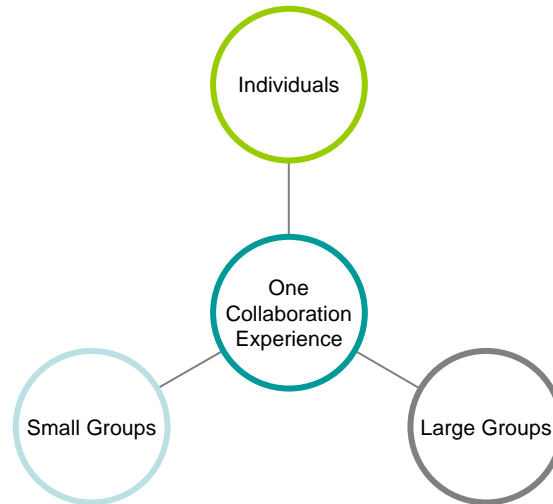
Cost: Less than \$10,000 (CA)

**Small Group Projected Environment**  
(2-10 people)



Cost: \$25,000 - \$100,000 (CA)

## Institutional Requirements (Scalable Investment)

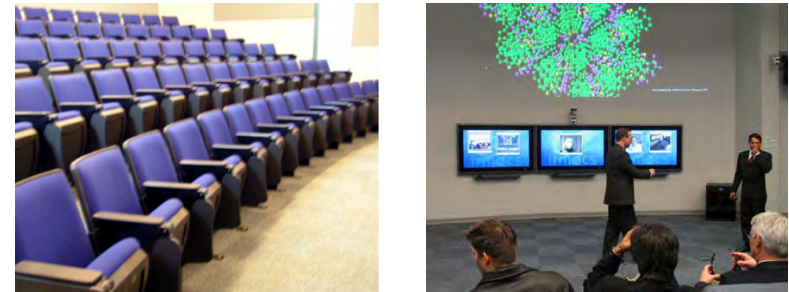


**Meeting Room Interactive Environment**  
(2-20 people)



Cost: \$150,000 (CA)

**Visualization Auditorium**



Cost: \$500,000+ (CA)

Six degrees of net separation ...



Being emulated by the Canadian Kandahar mission

I shall now show a variety of uses of high performance computing and communicating as part of

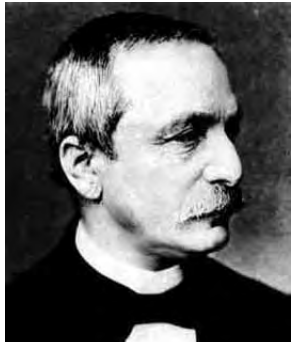
**Experimental Inductive Mathematics**

**Our web site:**

[www.experimentalmath.info](http://www.experimentalmath.info)

**contains all links and references**

AMS Notices  
Cover Article



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

Harold Edwards, *Essays in Constructive Mathematics*, 2004



# Caveman Geometry (2001)



Very cool for the **one** person with control



*"What I appreciate even more than its remarkable speed and accuracy are the words of understanding and compassion I get from it."*

# Outline. What is HIGH PERFORMANCE MATHEMATICS?

## 1b. Visual Data Mining in Mathematics.

- ✓ Fractals, Polynomials, Continued Fractions\*
- ✓ Pseudospectra and Code Optimization



## 2. High Precision Mathematics.

## 3. Integer Relation Methods.

- ✓ Chaos, Zeta\* and the Riemann Hypothesis
- ✓ Hex-Pi and Normality



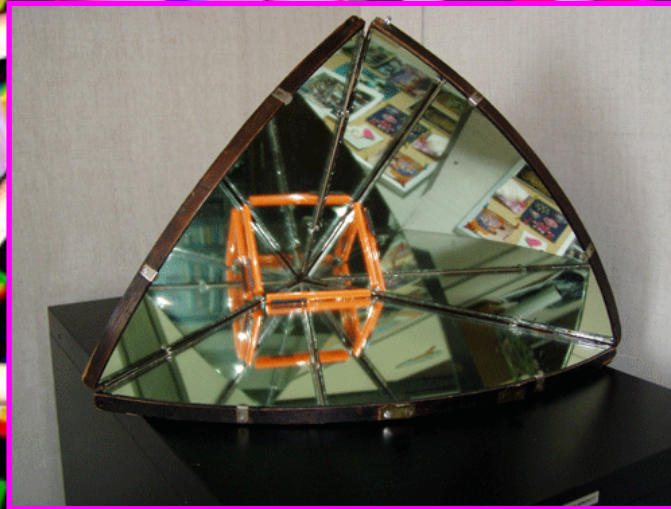
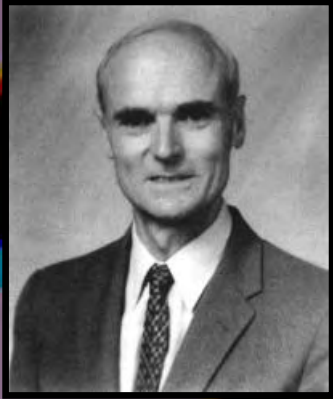
## 4. Inverse Symbolic Computation.

- ✓ A problem of Knuth\*,  $\pi/8$ , Extreme Quadrature

## 5. Demos and Conclusion.

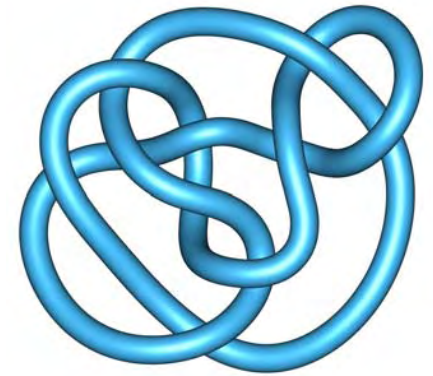
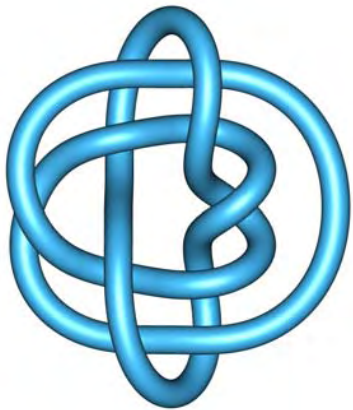
# COXETER'S (1927) Kaleidoscope

# Visualization



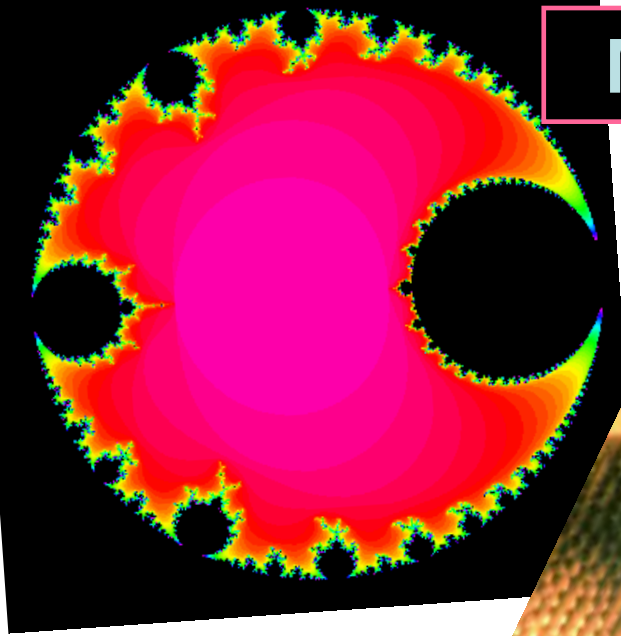
## The Perko Pair $10_{161}$ and $10_{162}$

are two adjacent 10-crossing knots (1900)



- first shown to be the same by Ken Perko in 1974
- and beautifully made dynamic in [KnotPlot](#) (open source)

# More Mathematical Data Mining



An unusual Mandelbrot parameterization

Various visual examples follow

- Indra's pearls
- Roots of  $x^2 - 1$  polynomials
- Ramanujan's fraction
- Sparsity and Pseudospectra



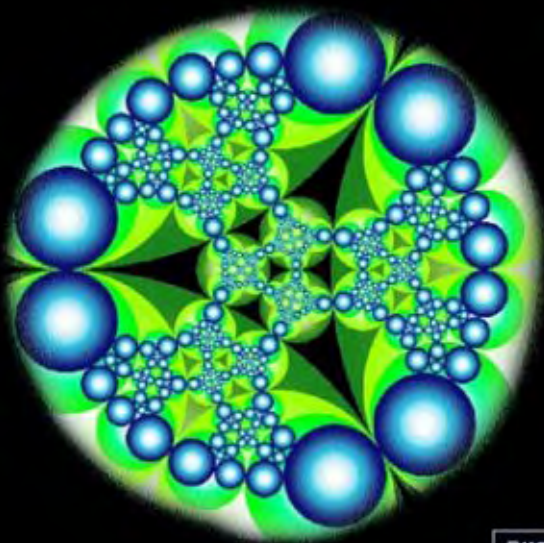
AK Peters, 2004  
(CD in press)

# Indra's Pearls

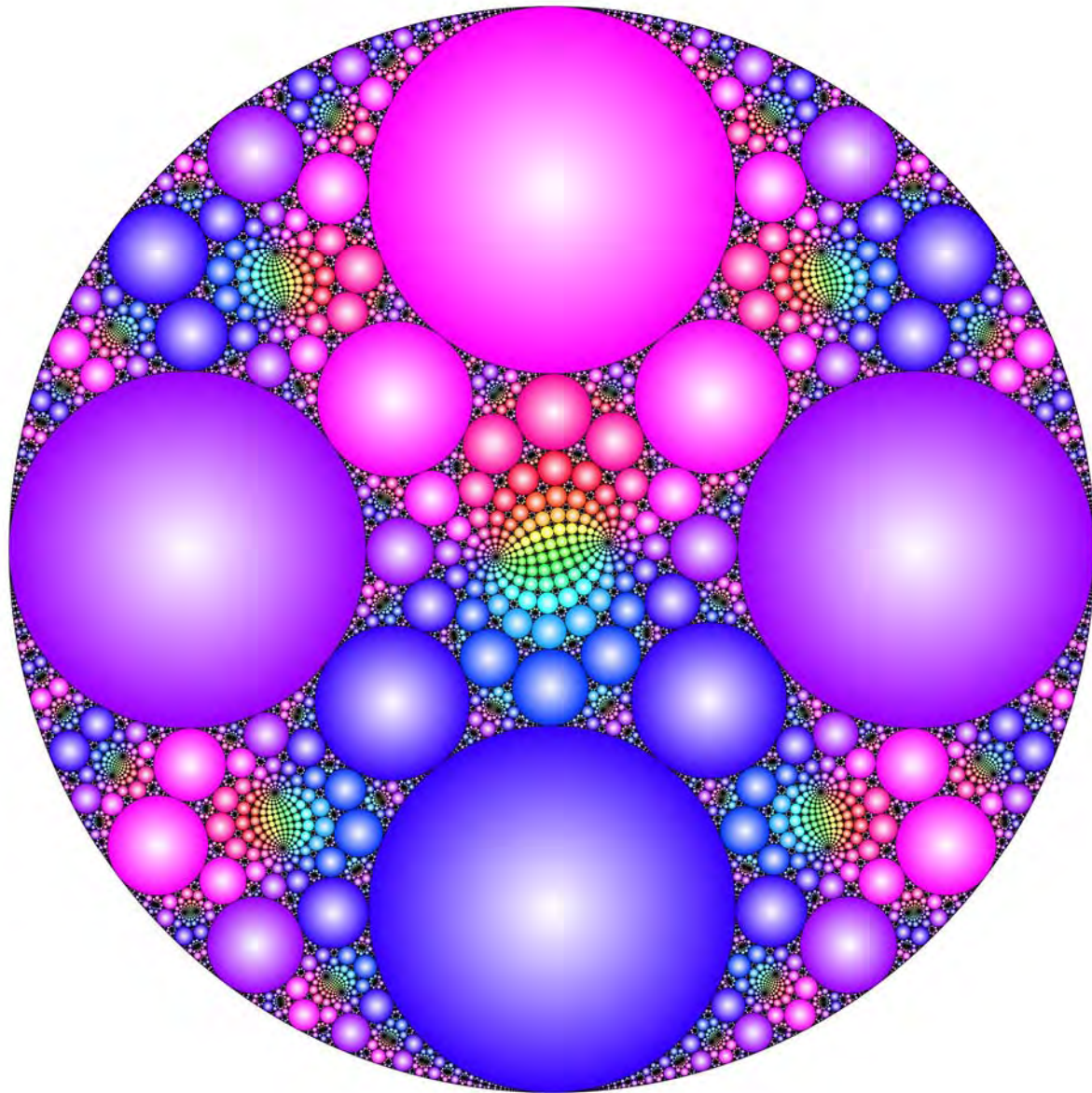
A merging of 19<sup>th</sup>  
and 21<sup>st</sup> Centuries

INDRA'S  
PEARLS The Vision of Felix Klein

David Mumford, Caroline Series, David Wright

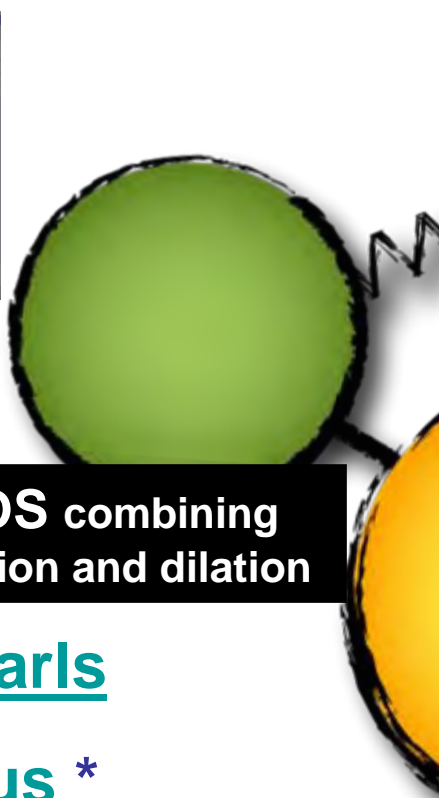
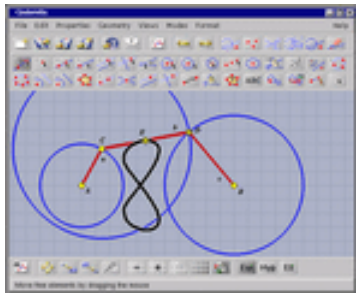


Double cusp group



2002: <http://klein.math.okstate.edu/IndrasPearls/>

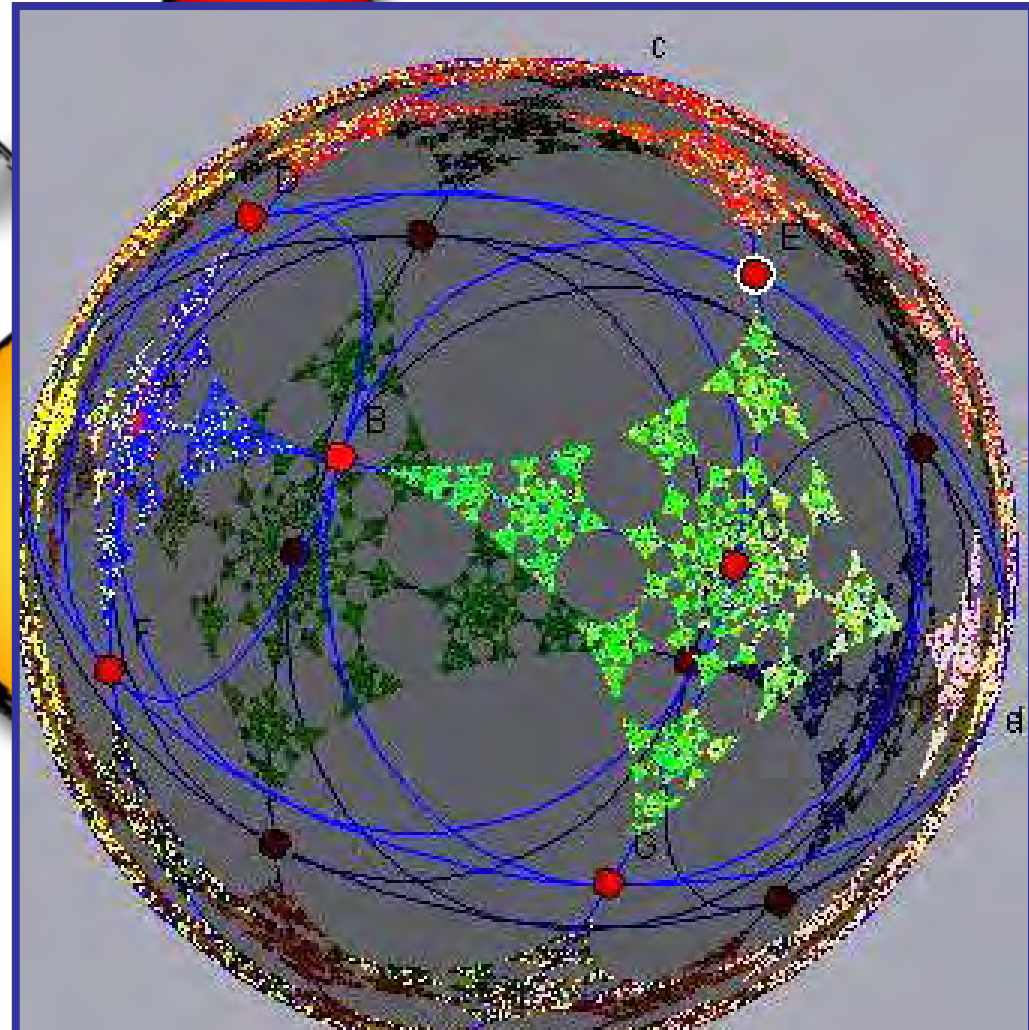
# CINDERELLA's dynamic geometry



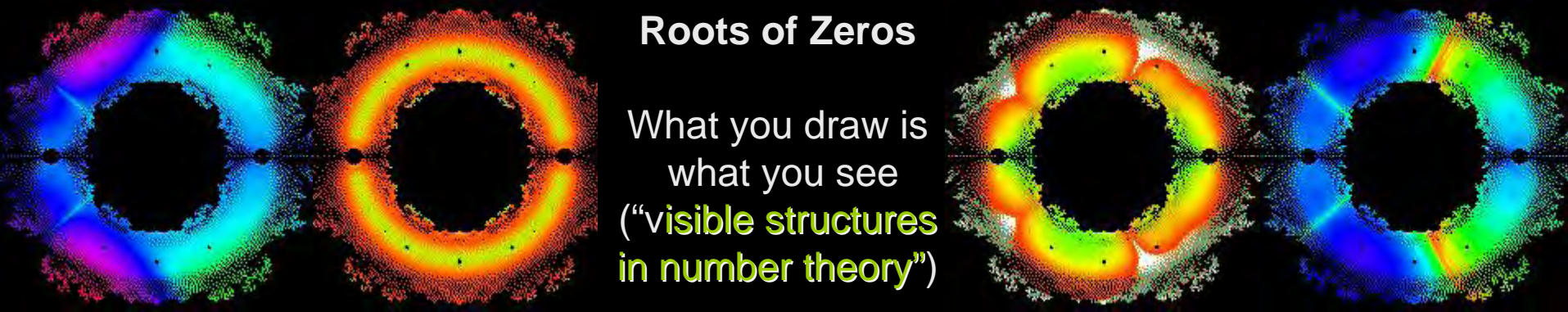
[www.cinderella.de](http://www.cinderella.de)

**FOUR DEMOS** combining inversion, reflection and dilation

1. [Indraspearls](#)
2. [Apollonius](#) \*
3. [Hyperbolicity](#)
4. [Gasket](#)







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

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

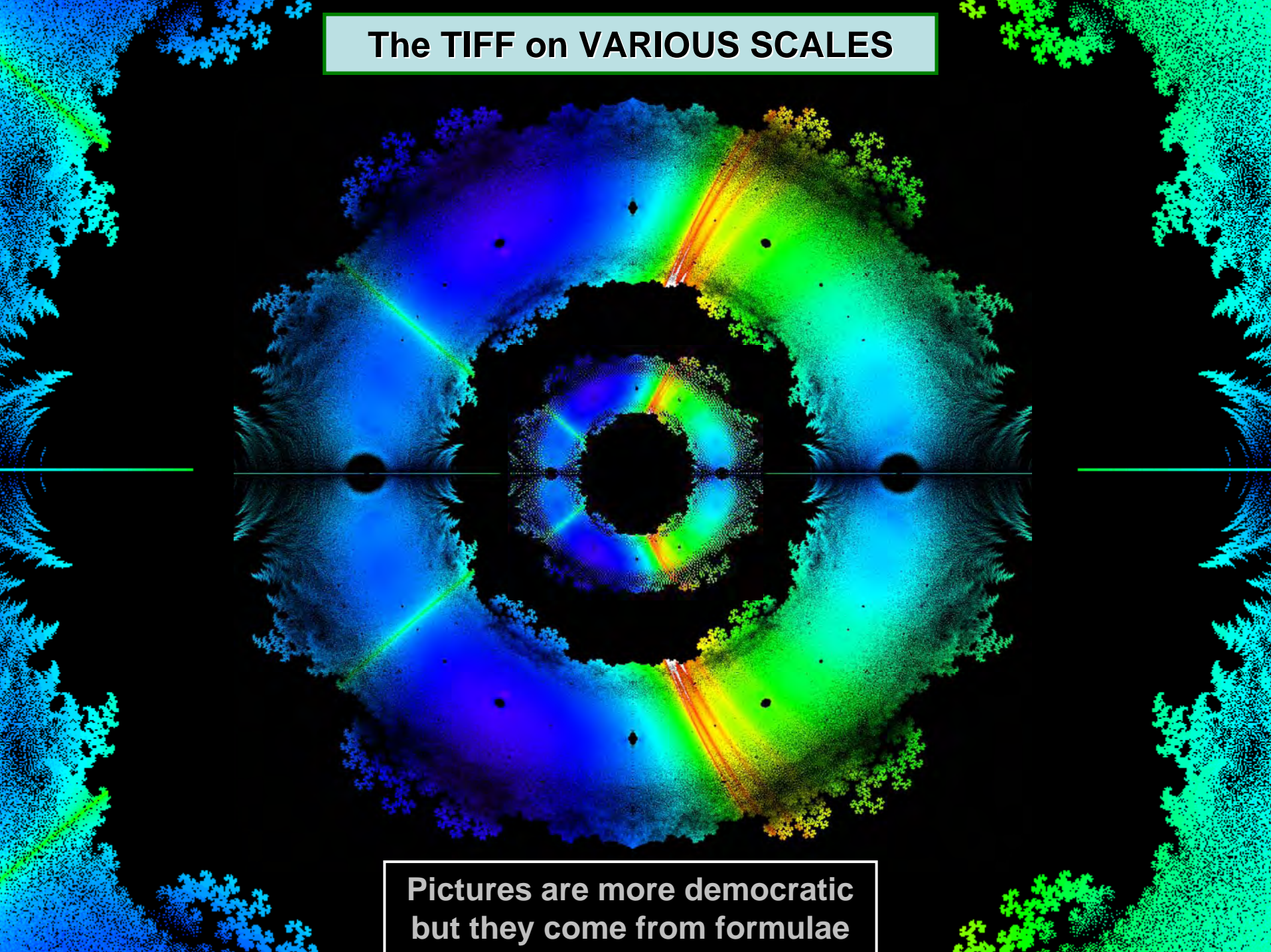
- All zeros are pictured (at **3600 dpi**)
- Figure 1b is colored by their local density
- Figure 1d shows sensitivity relative to the  $x^9$  term
- **The white and orange striations are not understood**

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

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

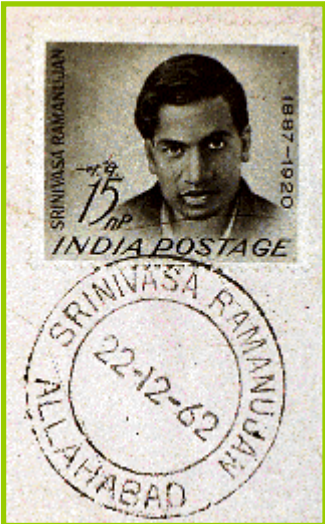
Greg Chaitin, [Interview](#), 2000.

# The TIFF on VARIOUS SCALES



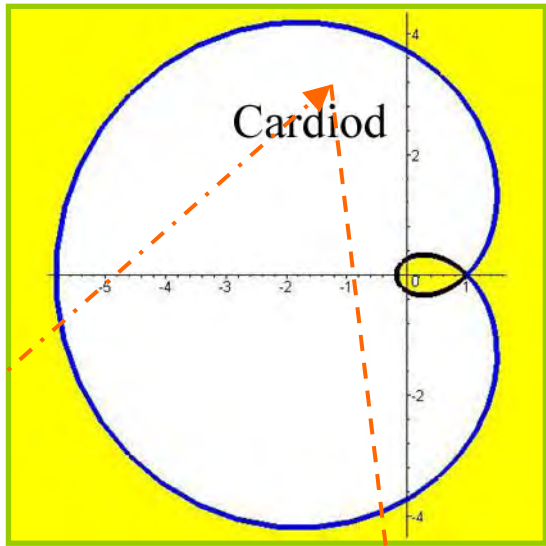
Pictures are more democratic  
but they come from formulae





# Ramanujan's Arithmetic-Geometric Continued fraction (CF)

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



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

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

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

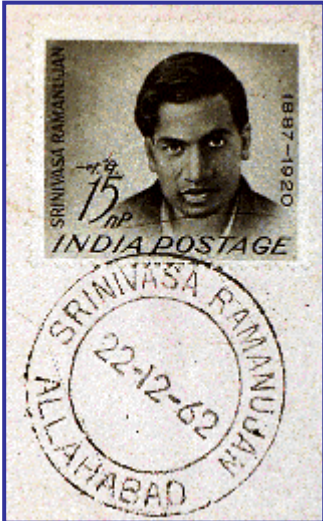
We wished to know for which  $a/b$  in  $\mathbb{C}$  this all held

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

Which discovery it remained to prove?

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

# Ramanujan's Arithmetic-Geometric Continued fraction

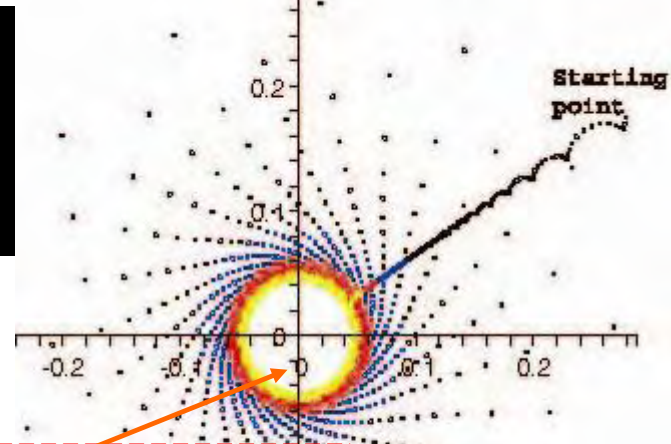


## 1. The Blackbox

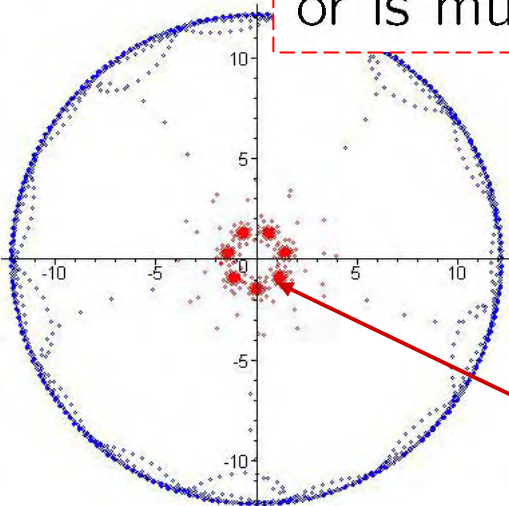
Six months later we had a beautiful proof using genuinely new dynamical results. Starting from the dynamical system  $t_0 := t_1 := 1$ :

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

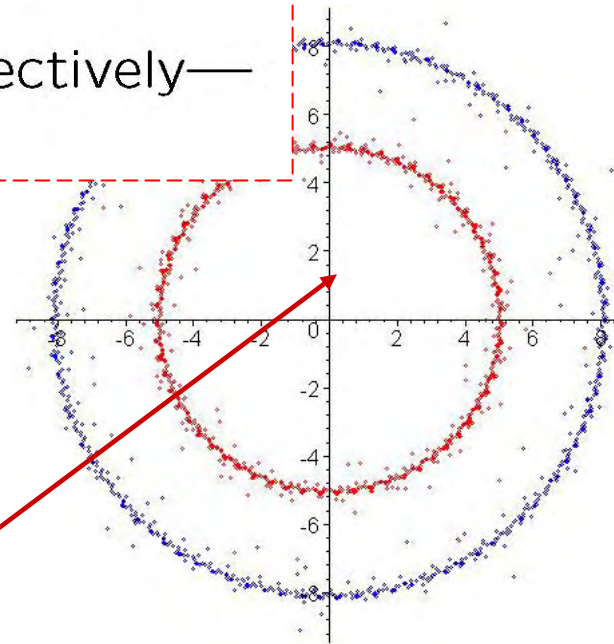
where  $\omega_n = a^2, b^2$  for  $n$  even, odd respectively—or is much more general.\*



## 2. Seeing convergence



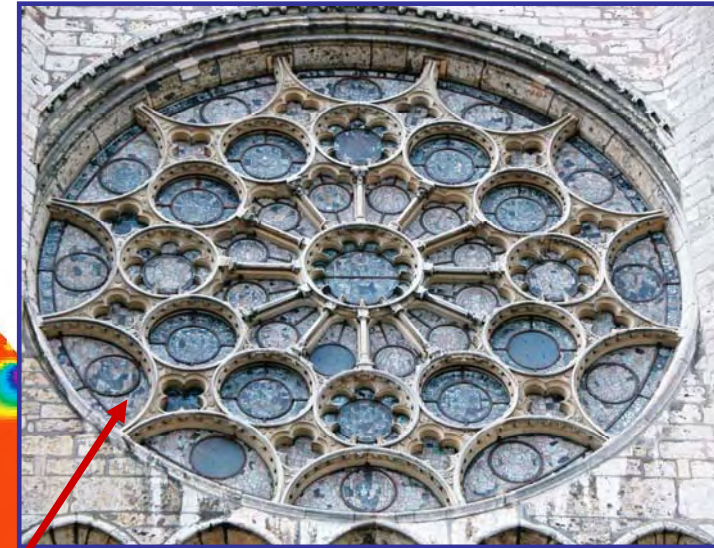
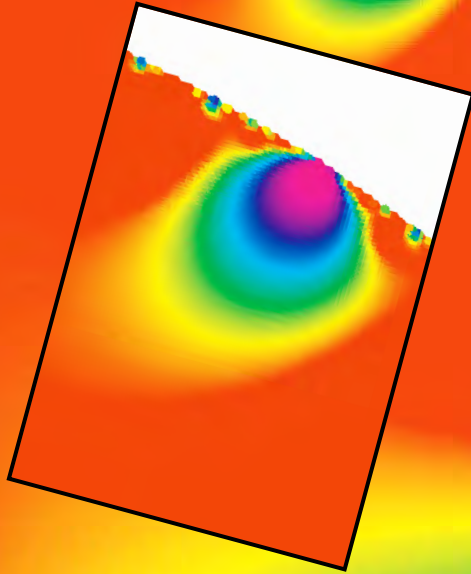
## 3. Attractors. Normalizing by $n^{1/2}$ three cases appear



# Mathematics and the aesthetic

Modern approaches to an ancient affinity

(CMS-Springer, 2005)



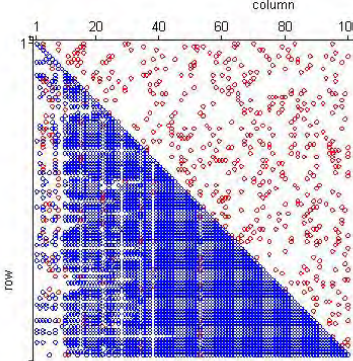
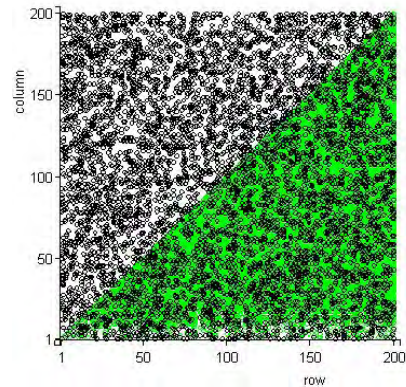
Why should I refuse a good dinner simply because I don't understand the digestive processes involved?

Oliver Heaviside  
(1850 - 1925)

✓ when criticized for his daring use of operators before they could be justified formally

# Pseudospectra or Stabilizing Eigenvalues

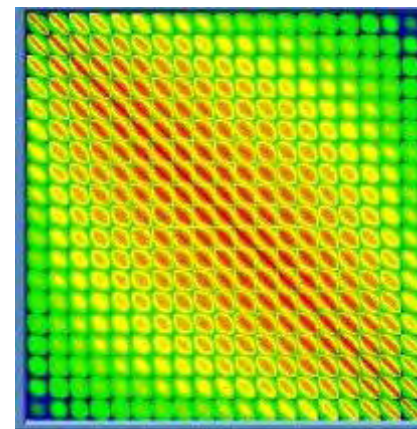
Gaussian elimination of random sparse (10%-15%) matrices



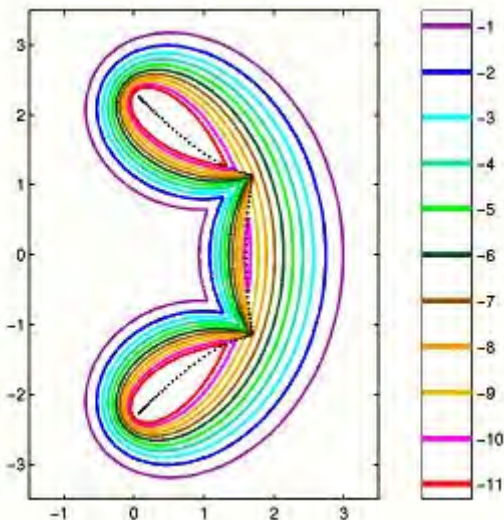
## 'Large' ( $10^5$ to $10^8$ ) Matrices must be seen

- ✓ conditioning and ill-conditioning
- ✓ sparsity and its preservation
- ✓ eigenvalues
- ✓ singular values (helping Google work)

A dense inverse



Pseudospectrum of a banded matrix

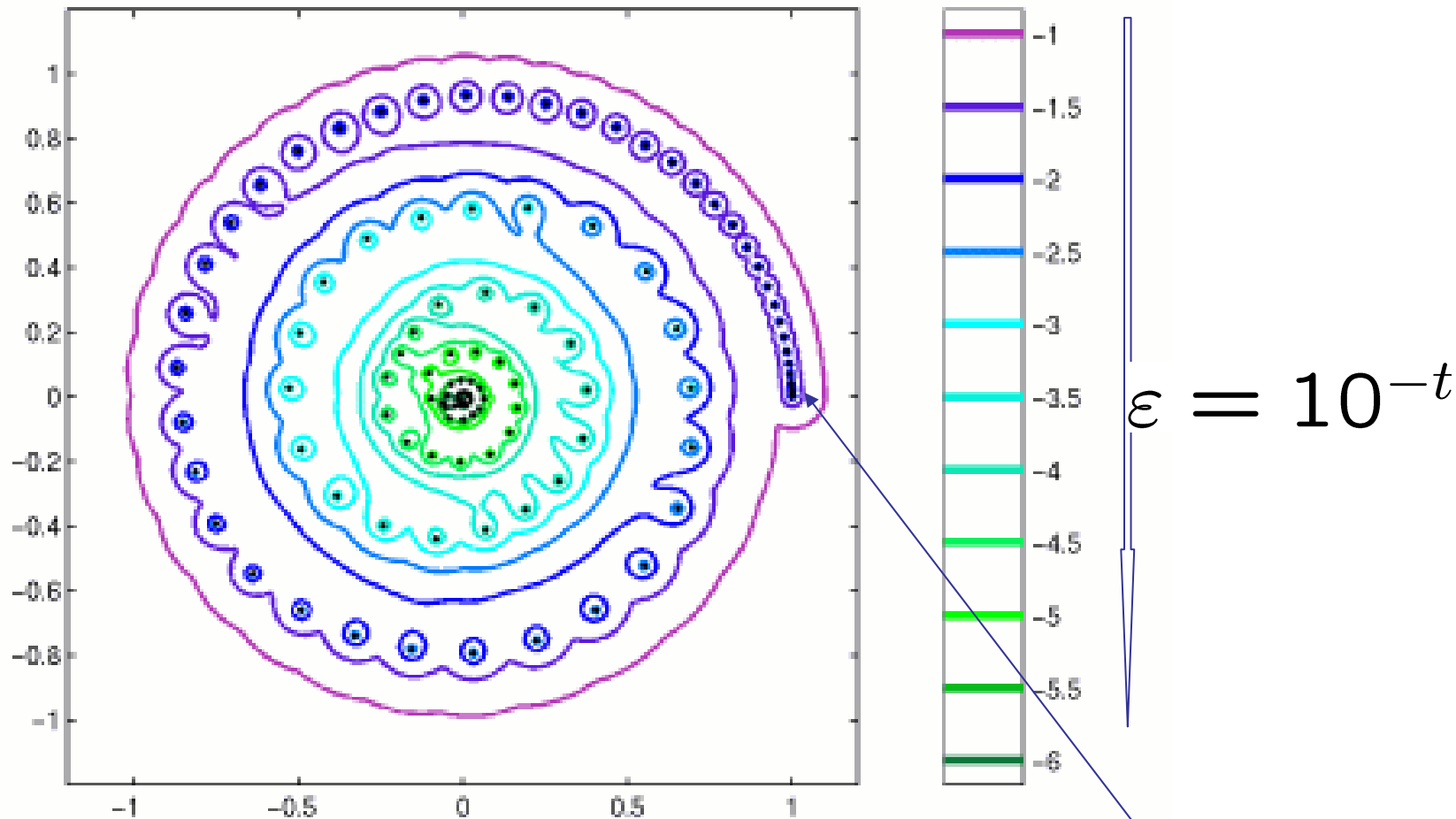


The pseudo spectrum of  $A$ : for  $\varepsilon > 0$

$$\sigma_\varepsilon(A) = \{ \lambda : \inf \|Ax - \lambda x\| \leq \varepsilon \}$$

<http://web.comlab.ox.ac.uk/projects/pseudospectra>

# An Early Use of Pseudospectra (Landau, 1977)



An infinite dimensional integral equation in laser theory

- ✓ discretized to a matrix of dimension **600**
- ✓ projected onto a well chosen invariant subspace of dimension **109**



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## 5. Demos and Conclusion.

## A WARMUP Computational Proof



Suppose we know that  $1 < N < 10$  and that  $N$  is an integer  
- **computing  $N$  to 1 significant place with a certificate** will  
prove the value of  $N$ . *Euclid's method* is basic to such ideas.

Likewise, suppose we know  $\alpha$  is algebraic of degree  $d$  and length  $\lambda$   
(coefficient sum in absolute value)

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

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

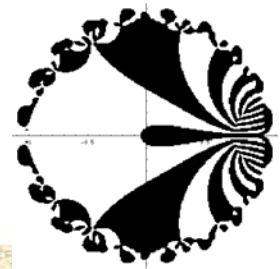
$$\int_{-\infty}^{\infty} \frac{y^2}{1 + 4y + y^6 - 2y^4 - 4y^3 + 2y^5 + 3y^2} dy = \pi$$

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

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

A fully symbolic Maple proof followed. **QED**  $|\beta - 1| < 1/(32\lambda) \mapsto \beta = 1$

# Numeric and Symbolic Computation



□ Central to my work - with Dave Bailey - meshed with visualization, randomized checks, many web interfaces and

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

## The On-Line Encyclopedia of Integer Sequences

Enter a  sequence,  word, or  sequence number:

1, 2, 3, 6, 11, 23, 47, 106, 235

Search

Restore example

[Clear](#)

[Hints](#)

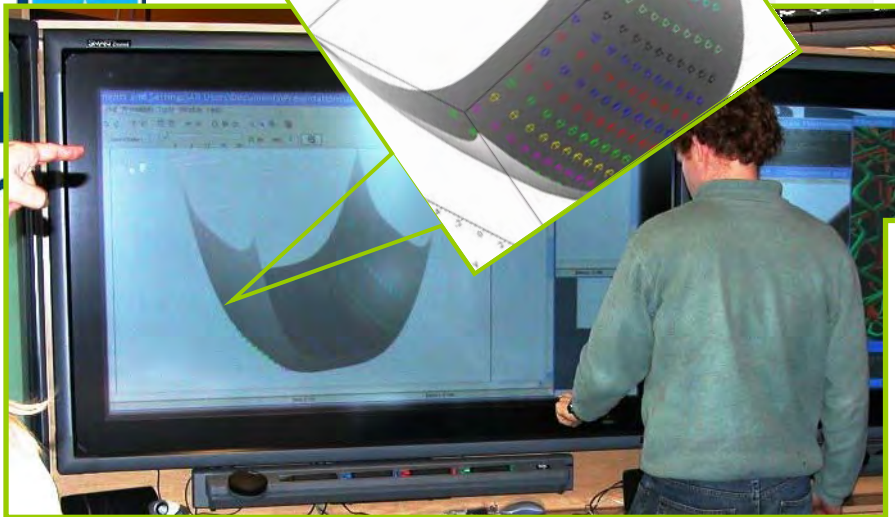
[Advanced look-up](#)

**Other languages:** [Albanian](#) [Arabic](#) [Bulgarian](#) [Catalan](#) [Chinese \(simplified, traditional\)](#) [Croatian](#) [Czech](#) [Danish](#) [Dutch](#) [Esperanto](#) [Estonian](#) [Finnish](#) [French](#) [German](#) [Greek](#) [Hebrew](#) [Hindi](#) [Hungarian](#) [Italian](#) [Japanese](#) [Korean](#) [Polish](#) [Portuguese](#) [Romanian](#) [Russian](#) [Serbian](#) [Spanish](#) [Swedish](#) [Tagalog](#) [Thai](#) [Turkish](#) [Ukrainian](#) [Vietnamese](#)

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[More pages](#) | [Superseeker](#) | Maintained by [N. J. A. Sloane](#) ([njas@research.att.com](mailto:njas@research.att.com))

[Last modified Fri Apr 22 21:18:02 EDT 2005. Contains 105526 sequences.]



*Parallel derivative free optimization in **Maple***

- Other useful tools :
- Parallel Maple
  - Sloane's online sequence database
  - Salvy and Zimmermann's generating function package '*gfun*'
    - Automatic identity proving: Wilf-Zeilberger method for hypergeometric functions



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

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

## An Exemplary Database

**ID Number:** A000055 (Formerly MO791 and NO299)

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

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

**Name:** Number of trees with n unlabeled nodes.

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

**References** F. Bergeron, G. Labelle and P. Leroux, *Combinatorial Species and Tree-Like Structures*, Camb. 1998, p. 279.

N. L. Biggs et al., *Graph Theory 1736-1936*, Oxford, 1976, p. 49.

S. R. Finch, *Mathematical Constants*, Cambridge, 2003, pp. 295-316.

D. D. Grant, The stability index of graphs, pp. 29-52 of *Combinatorial Mathematics (Proceedings 2nd Australian Conf.)*, Lect. Notes Math. 403, 1974.

F. Harary, *Graph Theory*. Addison-Wesley, Reading, MA, 1969, p. 232.

F. Harary and E. M. Palmer, *Graphical Enumeration*, Academic Press, NY, 1973, p. 58 and 244.

D. E. Knuth, *Fundamental Algorithms*, 3d Ed. 1997, pp. 386-88.

R. C. Read and R. J. Wilson, *An Atlas of Graphs*, Oxford, 1998.

J. Riordan, *An Introduction to Combinatorial Analysis*, Wiley, 1958, p. 138.

**Links:** P. J. Cameron, [Sequences realized by oligomorphic permutation groups](#) *J. Integ. Seqs. Vol.*

Steven Finch, [Otter's Tree Enumeration Constants](#)

E. M. Rains and N. J. A. Sloane, [On Cayley's Enumeration of Alkanes \(or 4-Valent Trees\)](#),

N. J. A. Sloane, [Illustration of initial terms](#)

E. W. Weisstein, [Link to a section of The World of Mathematics](#).

[Index entries for sequences related to trees](#)

[Index entries for "core" sequences](#)

G. Labelle, C. Lamathe and P. Leroux, [Labeled and unlabeled enumeration of k-gonal 2-tr](#)

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



## Integrated real time use

- moderated

- 120,000 entries

- grows daily

- AP book had 5,000



# Fast Arithmetic (Complexity Reduction in Action)



## Multiplication

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

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

- The other operations

via Newton's method  $\times, \div, \sqrt{\cdot}$

- Elementary and special functions

via Elliptic integrals and Gauss AGM

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

## For example:

Karatsuba  
replaces one  
'times' by  
many 'plus'

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

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

# Ising Integrals (Jan 2006)

The following integrals arise in Ising theory of mathematical physics:

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

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

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

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

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

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

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

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



"What it comes down to is our software is too hard and our hardware is too soft."

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

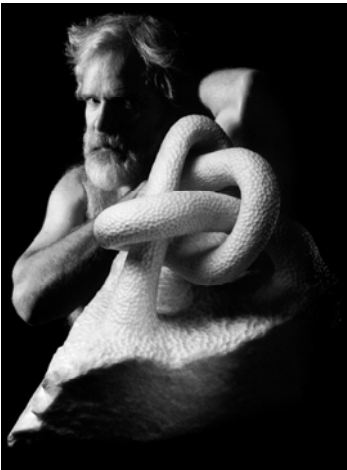
$$a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0$$

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

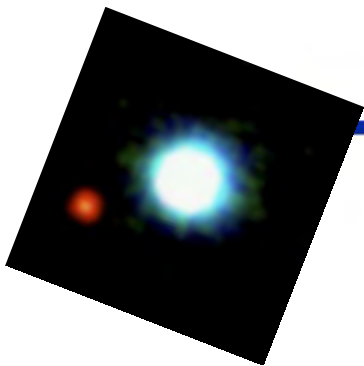
### An Immediate Use

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

Combinatorial optimization for pure mathematics (also LLL)



# Application of PSLQ: Bifurcation Points in Chaos Theory



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

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

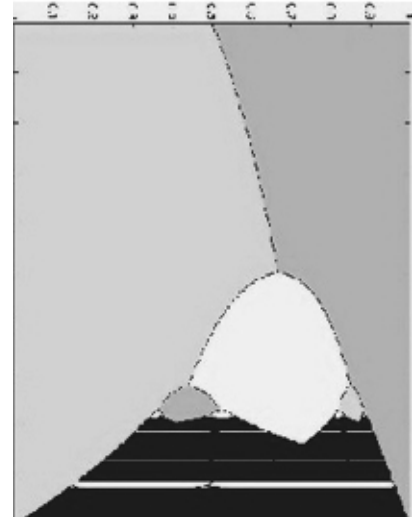
i.e.,  $B_3$  is the smallest  $r$  such that the iteration exhibits 8-way periodicity instead of 4-way periodicity.

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

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

Recently  $B_4$  was identified as the root of a 256-degree polynomial by a much more challenging computation. These results have subsequently been proven formally.

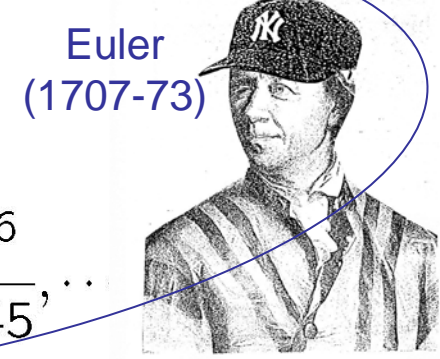
- The proofs use **Groebner basis techniques**
- Another useful part of the HPM toolkit





# PSLQ and Zeta

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

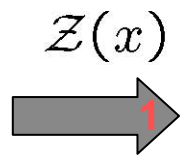


Euler  
(1707-73)

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

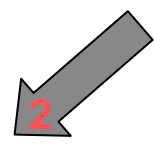
$$= \frac{\pi^2}{6}, \zeta(4) = \frac{\pi^4}{90}, \zeta(6) = \frac{\pi^6}{945}, \dots$$

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

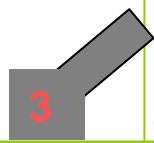


$$\begin{aligned} \mathcal{Z}(x) &= 3 \sum_{k=1}^{\infty} \frac{1}{\binom{2k}{k} (k^2 - x^2)} \prod_{n=1}^{k-1} \frac{4x^2 - n^2}{x^2 - n^2} \\ &= \sum_{k=0}^{\infty} \zeta(2k + 2) x^{2k} = \sum_{n=1}^{\infty} \frac{1}{n^2 - x^2} \end{aligned}$$

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



2. reduced as hoped

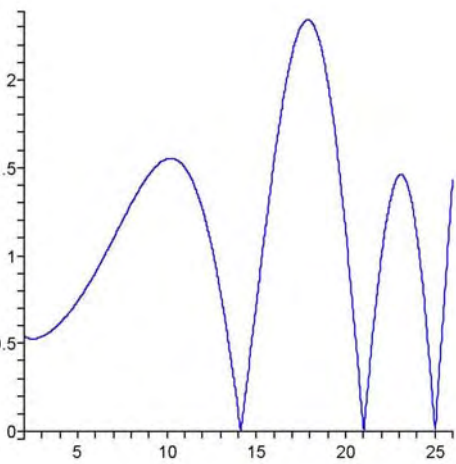


$$3n^2 \sum_{k=n+1}^{2n} \frac{\prod_{m=n+1}^{k-1} \frac{4n^2 - m^2}{n^2 - m^2}}{\binom{2k}{k} (k^2 - n^2)} = \frac{1}{\binom{2n}{n}} - \frac{1}{\binom{3n}{n}}$$

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

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

# Visualizing the Riemann Hypothesis (A Millennium Problem)

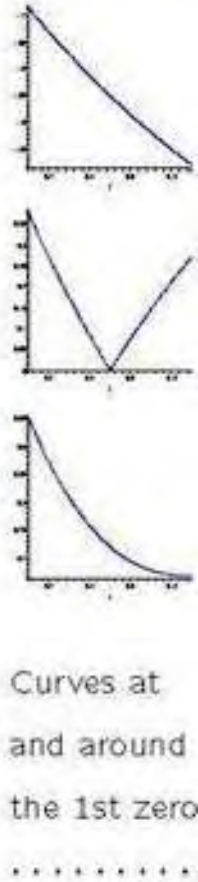
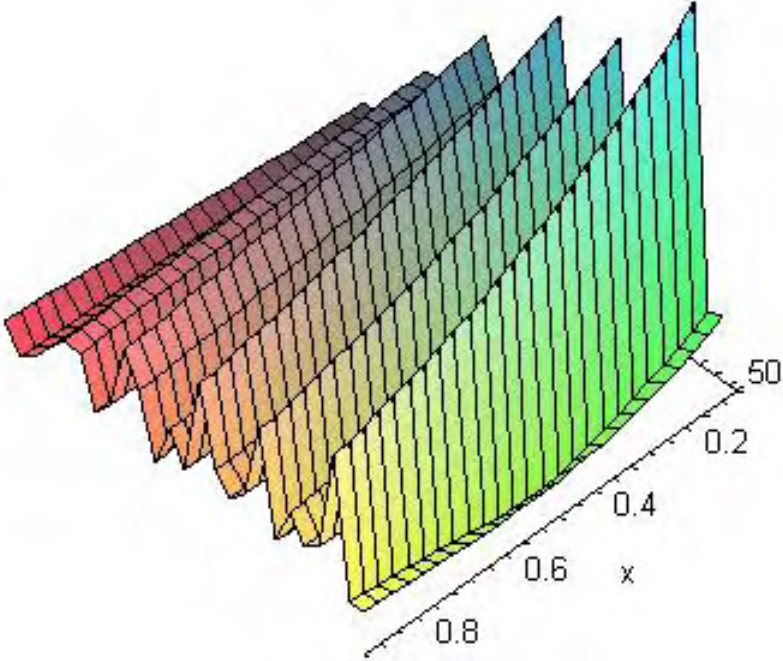


The imaginary parts of first 4 zeroes are:

14.134725142  
21.022039639  
25.010857580  
30.424876126

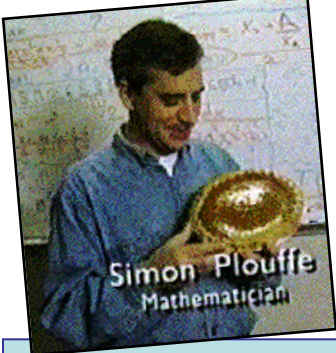
The first 1.5 billion are on the *critical line*

Yet at  $10^{22}$  the “**Law of small numbers**” still rules (Odlyzko)



**‘All non-real zeros have real part one-half’**  
(The Riemann Hypothesis)

Note the **monotonicity** of  $x \mapsto |\zeta(x+iy)|$  is **equivalent to RH** discovered in a Calgary class in 2002  
by Zvengrowski and Saidak



## PSLQ and Hex Digits of Pi

Finalist for the \$100K **Edge of Computation Prize** won by David Deutsch

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



My brother made the observation that this log formula allows one to compute binary digits of  $\log 2$  *without*

# Edge The Third Culture

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[Features](#)

[Edge Editions](#)

[Press](#)

[The Reality Club](#)

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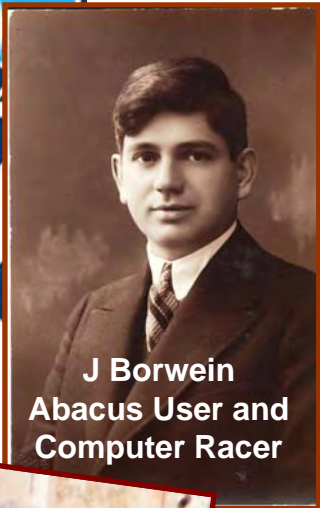
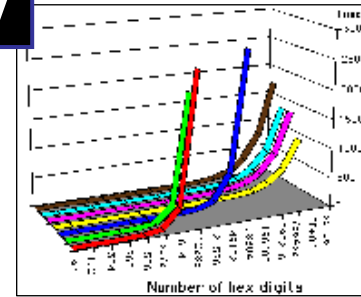
## THE \$100,000 EDGE OF COMPUTATION SCIENCE PRIZE

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

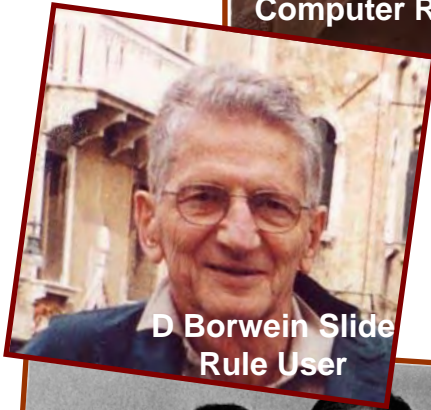
The Edge of Computation Science Prize, established by Edge Foundation, Inc., is a \$100,000 prize initiated and funded by science philanthropist Jeffrey Epstein.

# The pre-designed Algorithm ran the next day

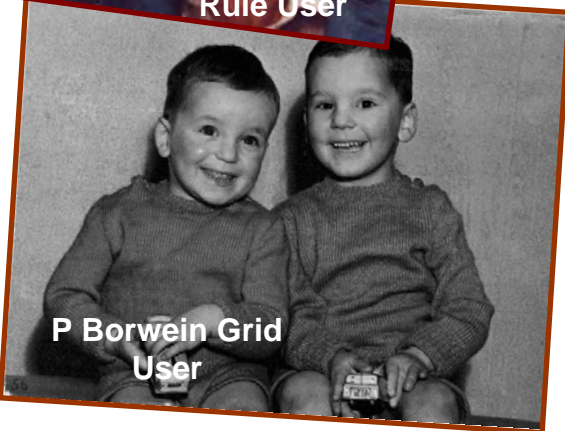
## ALGORITHMIC PROPERTIES



J Borwein  
Abacus User and  
Computer Racer



D Borwein Slide  
Rule User



P Borwein Grid  
User



T Borwein  
Game Player

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

Now built into some compilers!

(2) is implementable on any modern computer;

(3) requires no multiple precision software;

(4) requires very little memory; and

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

- [Join PiHex](#)
- [Download](#)
- [Source Code](#)
- [About](#)
- [Credits](#)
- [Status](#)
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- [What's New?](#)
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# PiHex

A distributed effort to calculate Pi.

The Quadrillionth Bit of Pi is '0'!  
The Forty Trillionth Bit of Pi is '0'!  
The Five Trillionth Bit of Pi is '0'!

Percival 2004



PiHex was a distributed computing project which used idle computing power to set three records for calculating specific bits of Pi. PiHex has now finished.

174962

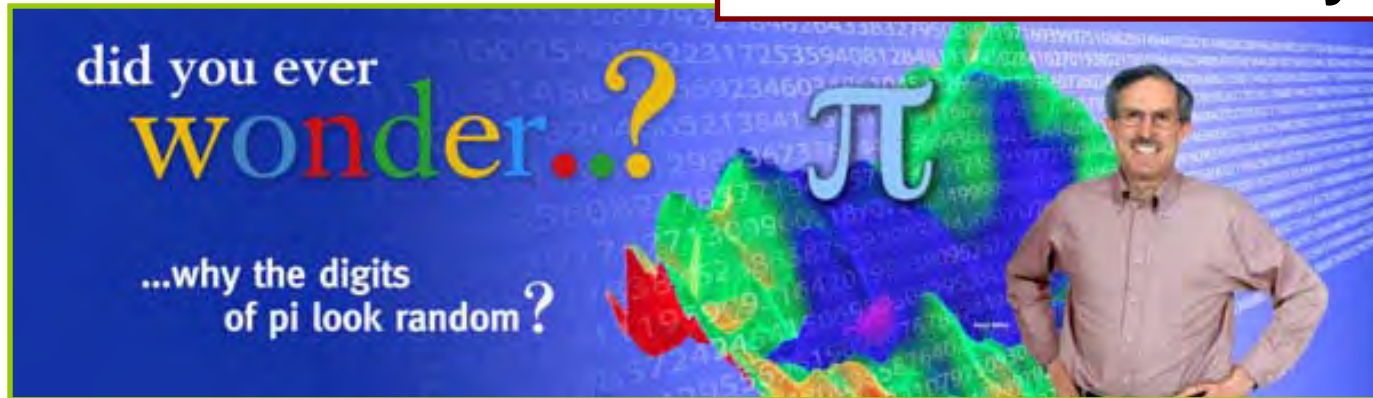
hits since the counter last reset.

Undergraduate  
**Colin Percival's**  
 grid computation  
**PiHex** rivaled  
**Finding Nemo**

Position	Hex Digits Beginning At This Position
$10^6$	26C65E52CB4593
$10^7$	17AF5863EFED8D
$10^8$	ECB840E21926EC
$10^9$	85895585A0428B
$10^{10}$	921C73C6838FB2
$10^{11}$	9C381872D27596
$1.25 \times 10^{12}$	07E45733CC790B
$2.5 \times 10^{14}$	E6216B069CB6C1

1999 on 1736 PCS  
 in 56 countries  
 using 1.2 million  
 Pentium2 cpu-hours

# PSLQ and Normality of Digits



Bailey and Crandall observed that BBP numbers most probably are normal and make it precise with a hypothesis on the behaviour of a dynamical system.

- For example Pi is normal in Hexadecimal if the iteration below, starting at zero, is uniformly distributed in  $[0,1]$

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

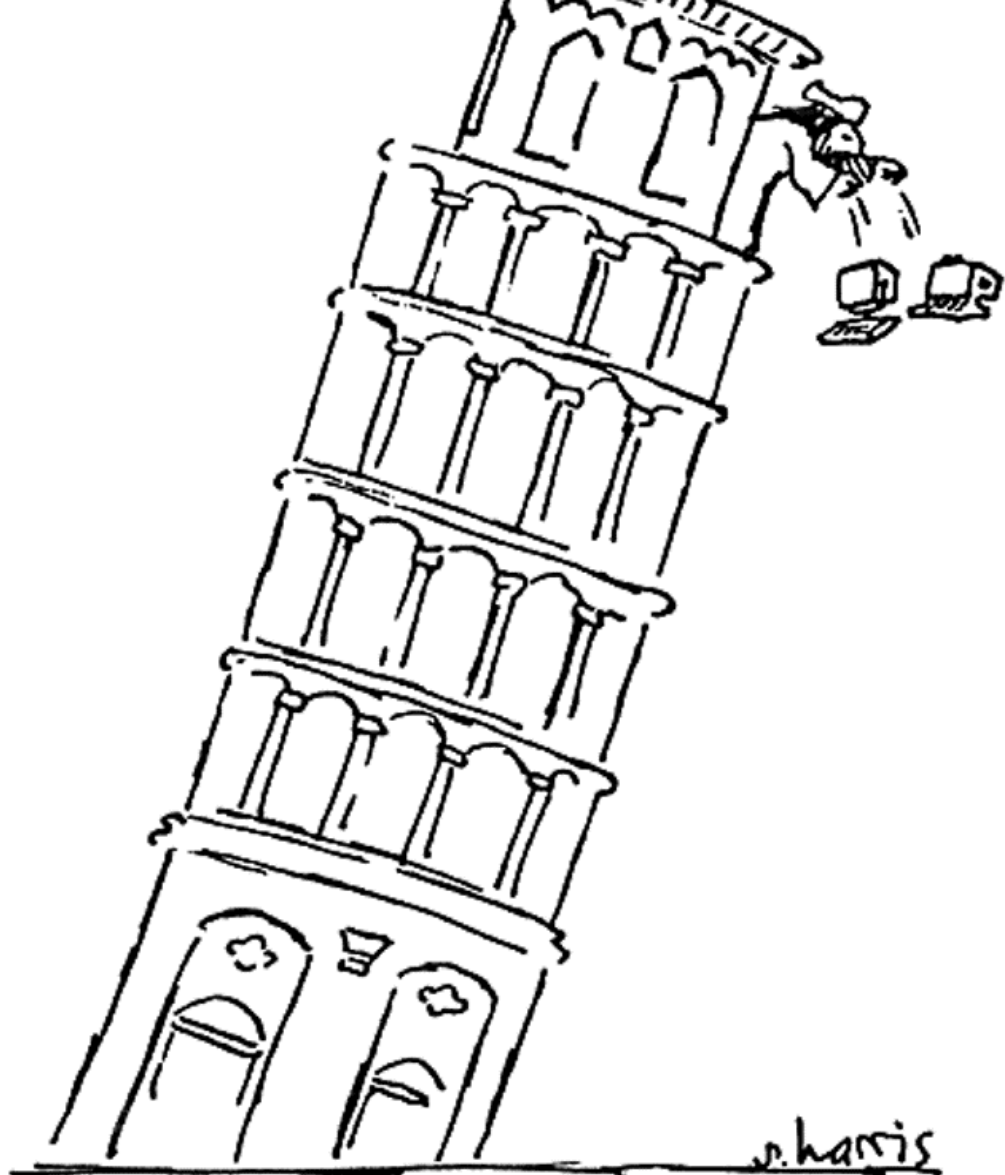
Consider the hex digit stream:

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

**We have checked this gives first million hex-digits of Pi**

Is this always the case? The weak Law of Large Numbers implies this is **very probably true!**





IF THERE WERE COMPUTERS  
IN GALILEO'S TIME

# Outline. What is HIGH PERFORMANCE MATHEMATICS?

## 1. Visual Data Mining in Mathematics.

- ✓ Fractals, Polynomials, Continued Fractions\*
- ✓ Pseudospectra and Code Optimization



## 2. High Precision Mathematics.

## 3. Integer Relation Methods.

- ✓ Chaos, Zeta\* and the Riemann Hypothesis
- ✓ Hex-Pi and Normality

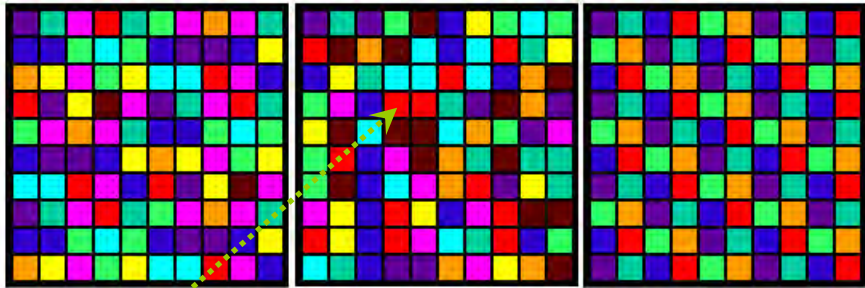


## 4. Inverse Symbolic Computation.

- ✓ A problem of Knuth\*,  $\pi/8$ , Extreme Quadrature

## 5. Demos and Conclusion.

# A Colour and an Inverse Calculator (1995)



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

## Inverse Symbolic Computation

### Inferring mathematical structure from numerical data

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

and **identify** in [Maple](#)

### INVERSE SYMBOLIC CALCULATOR

Please enter a number or a Maple expression:

Run  Clear

- Simple Lookup and Browser** for any number.
- Smart Lookup** for any number.
- Generalized Expansions** for real numbers of at least 16 digits.
- Integer Relation Algorithms** for any number.

Home ? Mail

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

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

**Input of  $\pi$**

Toggle View Toggle AutoSize

ROWS: 36 COLS: 36 MOD: 10 DIGIT: 0

3.141592653589793238462643  
0899862803482534211706798

3.14159265358979

STO RCL I J /

SIN 7 8 9 -

COS 4 5 6 +

TAN 1 2 3 \*

LOG 0 -

Edit

VARIABLE NAME: VARIABLE LIST:

VARIABLE VALUE:

C  
O  
L  
O  
R  
C  
A  
L  
C

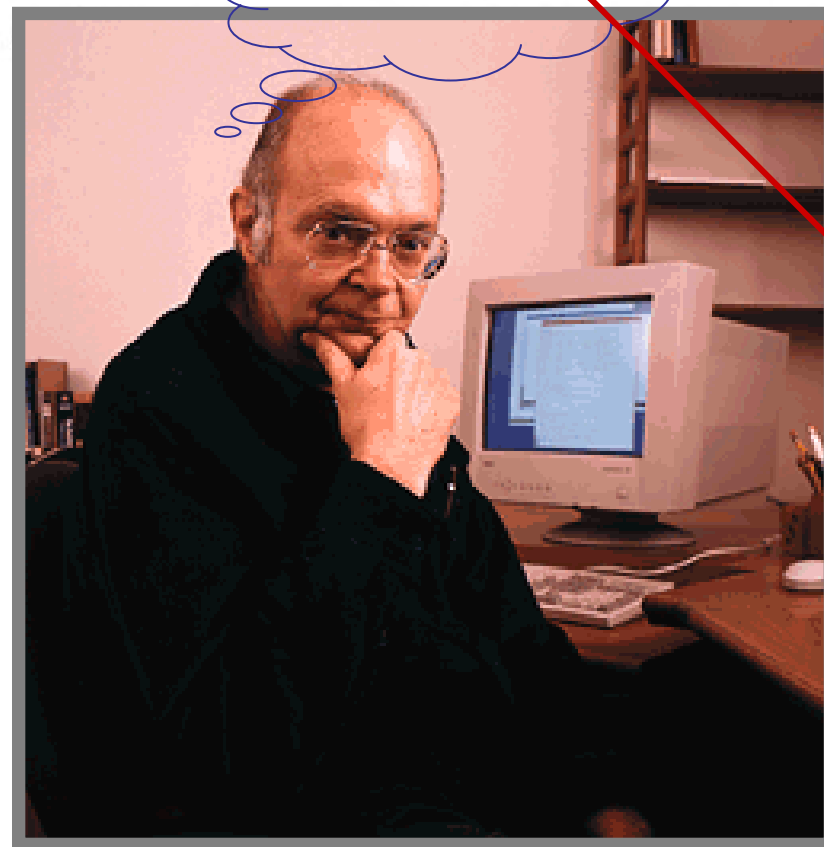
Expressions that are **not** numeric like  $\ln(\pi * \sqrt{2})$  are evaluated in [Maple](#) in symbolic form first, followed by a floating point evaluation followed by a lookup.

# Knuth's Problem

Donald Knuth\* asked for a closed form evaluation of:

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

“instrumentation”



te 20 or 200 digits

shown on next slide

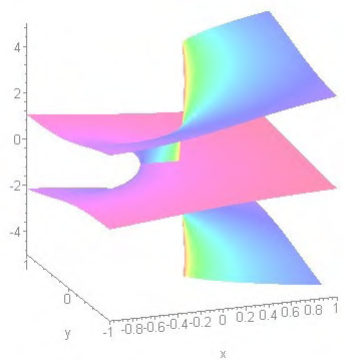
in the *Inverse Sym-*  
turns

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

which *Maple 9.5* on a  
in under 6 seconds

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

The answer is Gonnet's Lambert's W which solves  $W \exp(W) = x$



W's Riemann surface

\* ARGUABLY WE ARE DONE


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

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

**INVERSE SYMBOLIC CALCULATOR**

**TOP 5% OF ALL WEB SITES POINT**

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



**INVERSE SYMBOLIC CALCULATOR**

\_\_\_\_\_

Results of the search:

Maple output:

**.08406950872765600**

.8406950872765600e-1

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

\_\_\_\_\_

Performing a smart lookup on .8406950872765600e-1:

Function	Result	Precision	Matches
<b>K-2/3</b>	.58259715793901066666666666666666	16	1

**INVERSE SYMBOLIC CALCULATOR**

\_\_\_\_\_

579390106 was probably generated by one  
s or found in one of the given tables.

Answers are given from shortest to longest description

Mixed constants with 5 operations  
**5825971579390106 = Zeta(1/2)/sr(2)/sr(Pi)**

**Browse** around .5825971579390106.

# Quadrature I. Hyperbolic Knots



Dalhousie Distributed Research Institute and Virtual Environment

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

where

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

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

The easiest of 998 empirical results (PSLQ, PARI, SnapPea) linking physics/topology (LHS) to number theory (RHS).

[JMB-Broadhurst, 1996]

We have certain knowledge without proof

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



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

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

CPUs	Init	Integral #1	Integral #2	Total	Speedup
1	*190013	*1534652	*1026692	*2751357	1.00
16	12266	101647	64720	178633	15.40
64	3022	24771	16586	44379	62.00
256	770	6333	4194	11297	243.55
1024	199	1536	1034	2769	993.63

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

### Expected and unexpected scientific spinoffs

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



# Quadrature II. Ising Susceptibility Integrals

Bailey, Crandall and I are currently studying:

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

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

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

and

$$D_4 = \frac{7}{12}\zeta(3) = \frac{4}{9}\pi^2 - \frac{1}{6} - \frac{7}{2}\zeta(3)$$

- ✓ Computer Algebra Systems can (with help) find the first 3
- ✓  $D_4$  is a remarkable 1997 result due to McCoy--Tracy--Wu





# An Extreme Ising Quadrature

Recently Tracy asked for help 'experimentally' evaluating  $D_5$

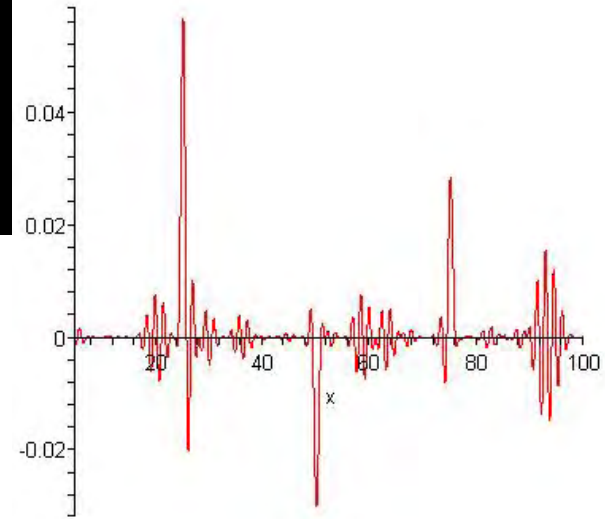
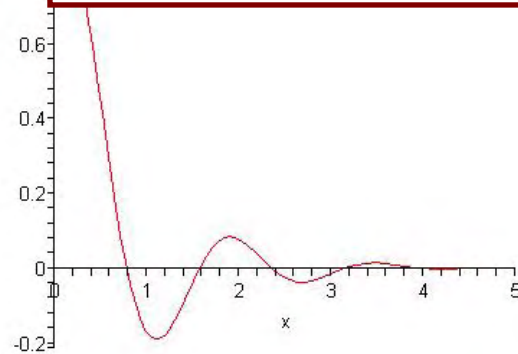
Using `PSLQ` this entails being able to evaluate a [five dimensional integral](#) to at least 50 or 250 places so that one can search for combinations of 6 to 15 constants

- ✓ Monte Carlo methods can certainly not do this
- ✓ We are able to reduce  $D_5$  to a horrifying several-page-long 3-D symbolic integral !
- ✓ **A 256 cpu `tanh-sinh` computation at LBNL provided 500 digits in 18.2 hours on `Bassi`, an IBM Power5 system:** **A FIRST**

0.00248460576234031547995050915390974963506067764248751615870769  
216182213785691543575379268994872451201870687211063925205118620  
699449975422656562646708538284124500116682230004545703268769738  
489615198247961303552525851510715438638113696174922429855780762  
804289477702787109211981116063406312541360385984019828078640186  
930726810988548230378878848758305835125785523641996948691463140  
911273630946052409340088716283870643642186120450902997335663411  
372761220240883454631501711354084419784092245668504608184468...

# Quadrature III. Pi/8?

A numerically  
challenging integral  
tamed



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

Now  $\pi/8$  equals

0.392699081698724154807830422909937860524645434

while the **integral** is

0.3926990816987241548078304229099378605246461749



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

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



Before and After

# REFERENCES



**Paseky,  
Merci a tous**



Enigma

Pla  
J.M  
Ex  
Dis  
D.H  
Ex  
So



Environment

ics by Experiment:  
A.K. Peters, 2003.

ohn,  
tational Paths to  
**Active CDs 2006]**

ntal Mathematics:  
optics Amer. Math.

*“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.

THE BIOCHEMIST  
AT WORK

A trace of  
saturated fat...  
very bad.

**SOME DEMOS  
FOLLOW**



THE BIOCHEMIST  
AT LUNCH

I'll have another  
order of fries.



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## 1. Visual Data Mining in Mathematics.

- ✓ Fractals, Polynomials, Continued Fractions\*
- ✓ Pseudospectra and Code Optimization



## 2. High Precision Mathematics.

## 3. Integer Relation Methods.

- ✓ Chaos, Zeta\* and the Riemann Hypothesis
- ✓ Hex-Pi and Normality



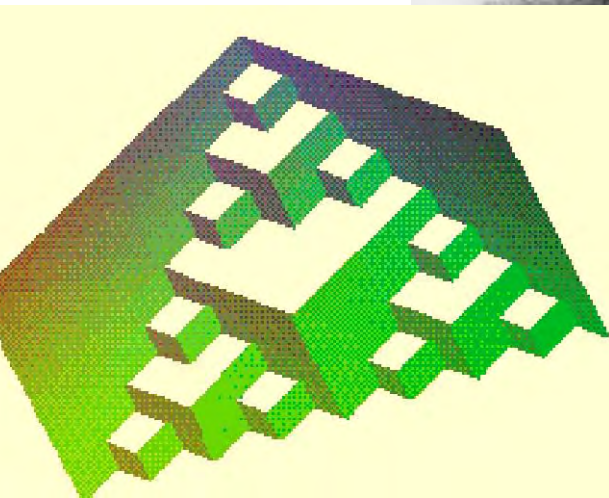
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- ✓ A problem of Knuth\*,  $\pi/8$ , Extreme Quadrature

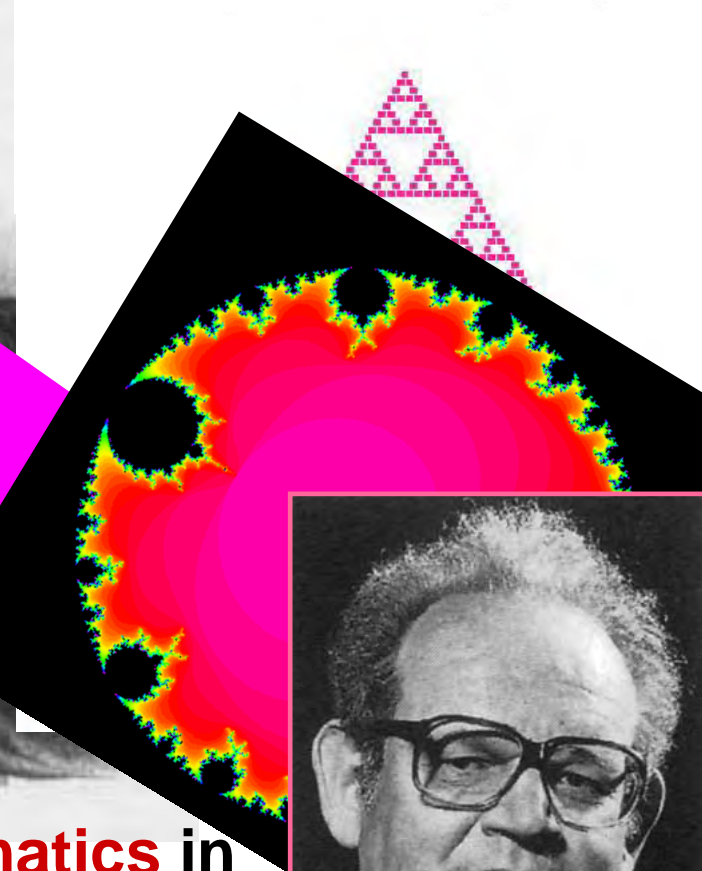
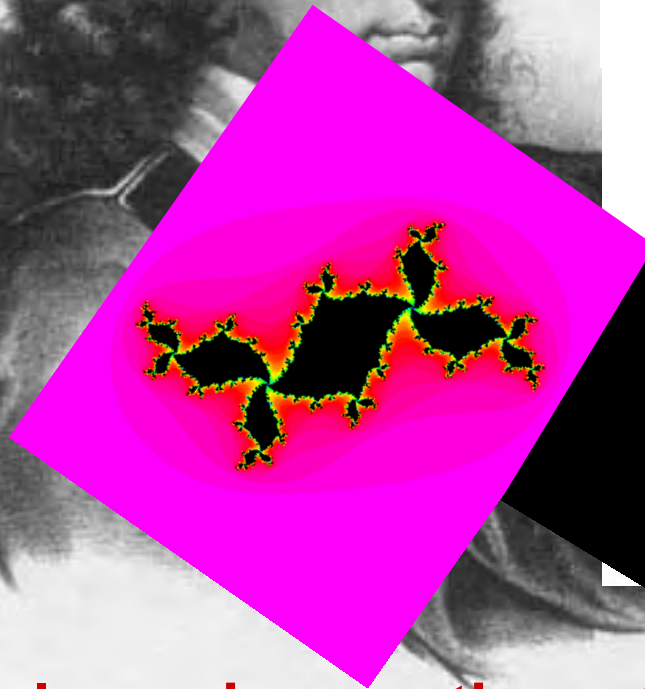
## 5. Demos and Conclusion.

# Inverse Systems and Self-Similarity everywhere

From **Pascal**  
and **Sierpinski**  
to **Julia**, **Fatou**  
& **Mandelbrot**



'cut and fold'



**Truly modern mathematics in  
nature, art and applications**

# Pascal's Triangle Interface

INSTRUCTIONS

[www.cecm.sfu.ca/interfaces](http://www.cecm.sfu.ca/interfaces)

Output Image

Rows (max 100):

30

Modulus (2 to 16):

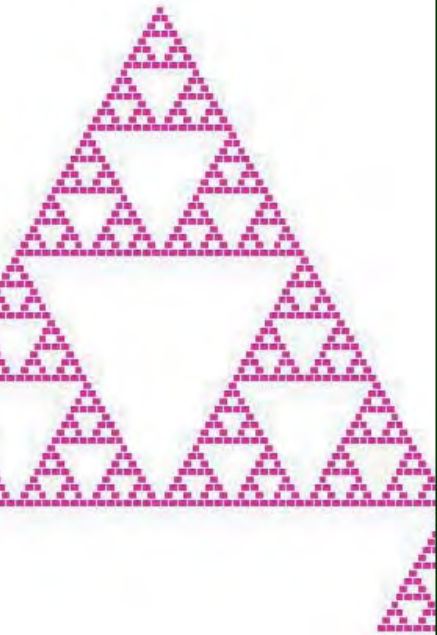
5

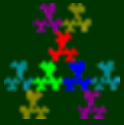
Image size:

300

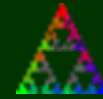
Deterministic and Random

```
1 11 1 2 1 1331 1 4 6 4 1 1 5 10 10 5 1
1 6 15 20 15 6 1 1 7 21 35 21 7 1
```





# FRACTALINA



## About Fractalina

Fractalina allows the input and iteration to play "the chaos game".

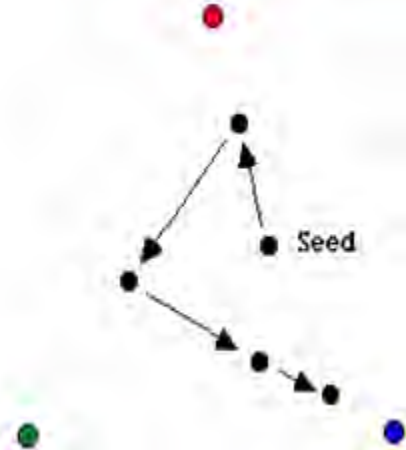
To see it in action, you can go directly to the Fractalina website.

The chaos game begins with the selection of a point. Each transformation has a special kind. Each transformation has a center point. Sometimes informally think of the point as a "seed". The transformations are of a special kind: they rotate or compress. We sometimes think of the point as a "seed". The transformations are of a special kind: they rotate or compress. We sometimes think of the point as a "seed".

The chaos game can be explained this way:

1. Starting at any point, randomly choose one of the transformations.
2. Go part of the way towards the center point of that transformation and rotate part way around it.
3. Repeat the process from the resulting point.

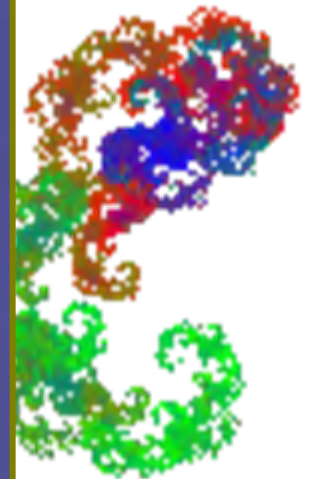
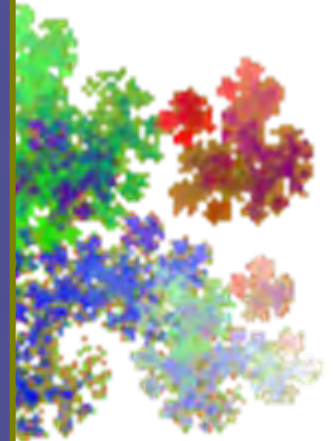
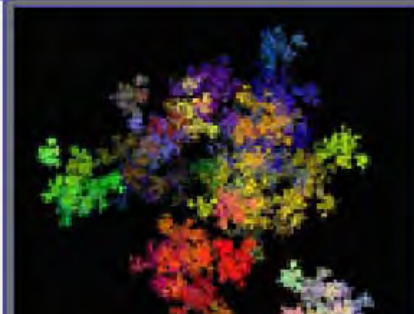
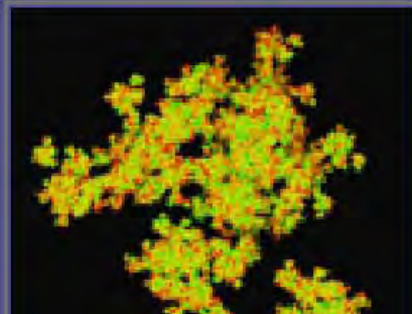
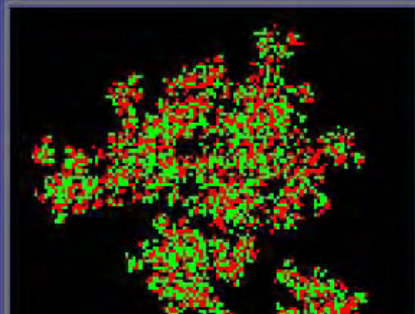
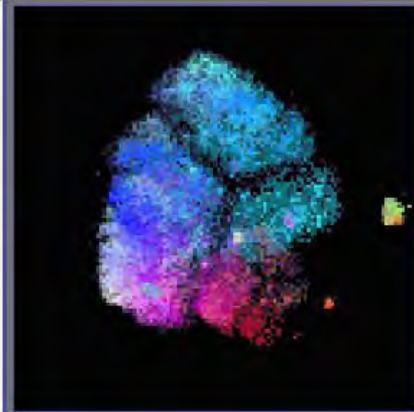
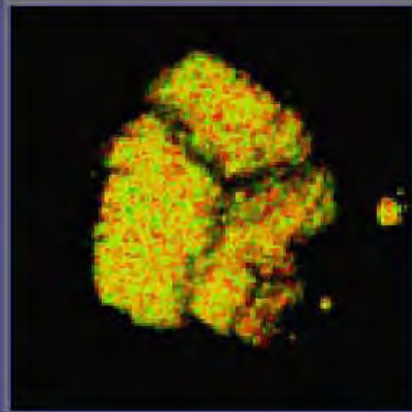
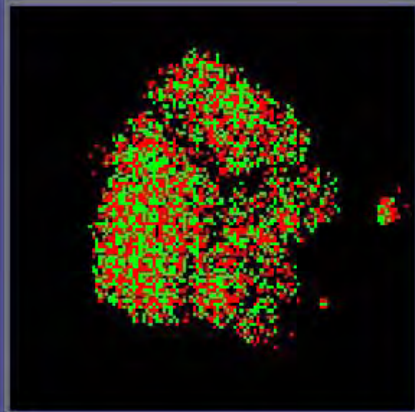
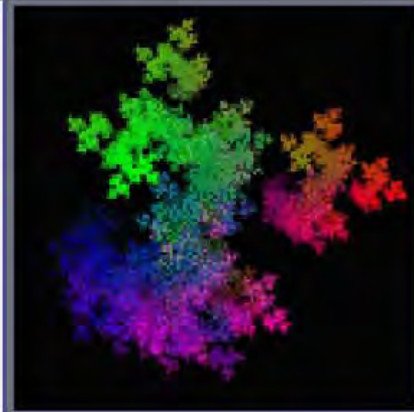
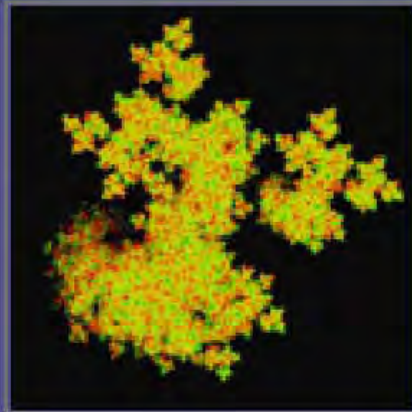
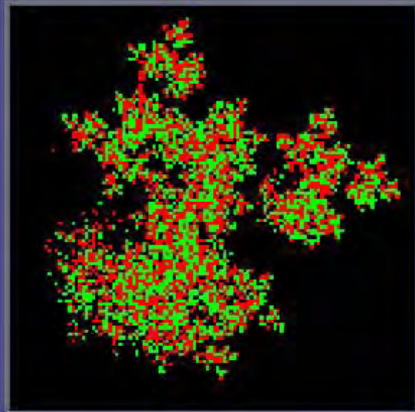
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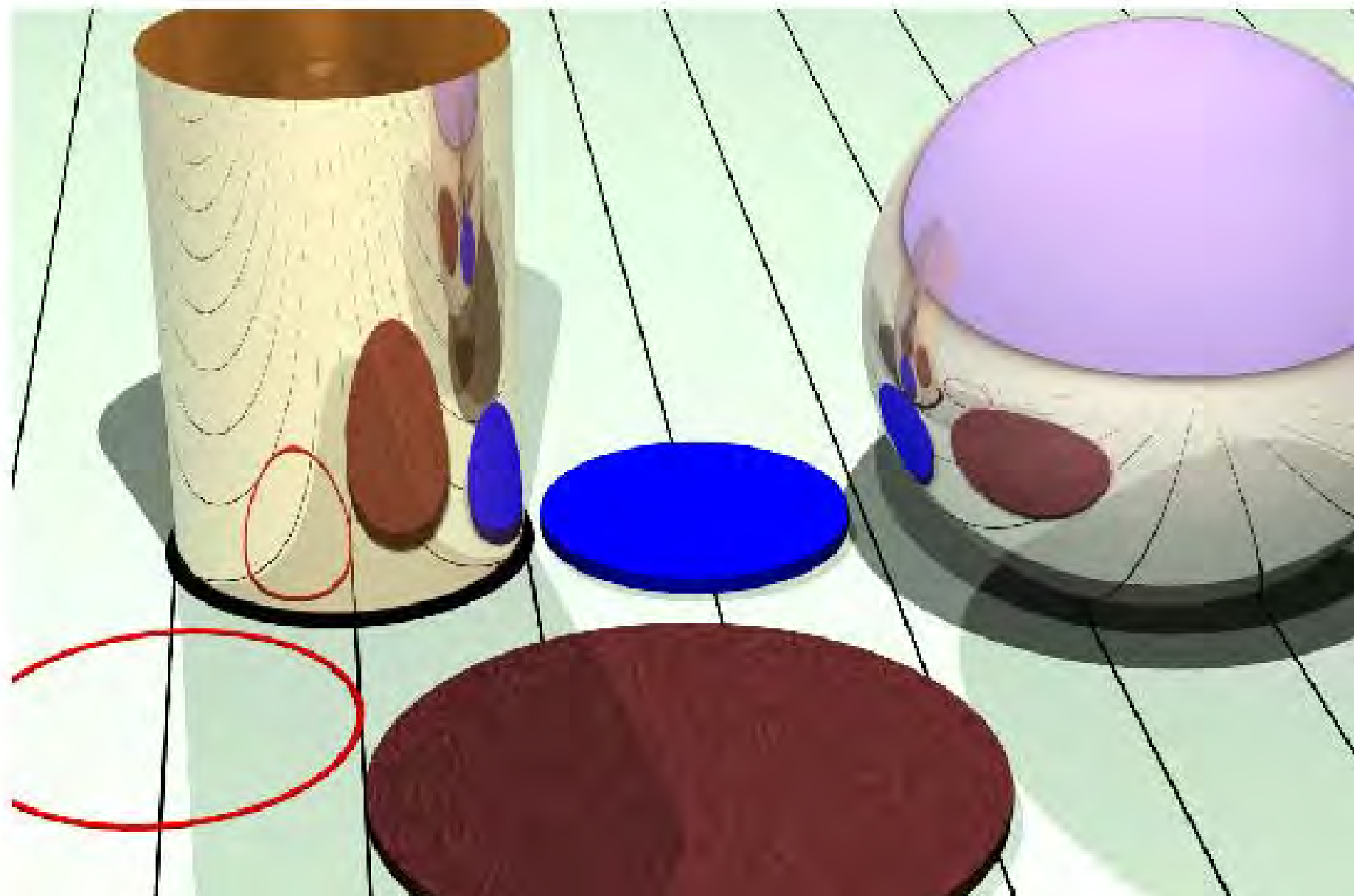
The transformations are of a special kind: they rotate or compress. We sometimes think of the point as a "seed". The transformations are of a special kind: they rotate or compress. We sometimes think of the point as a "seed".



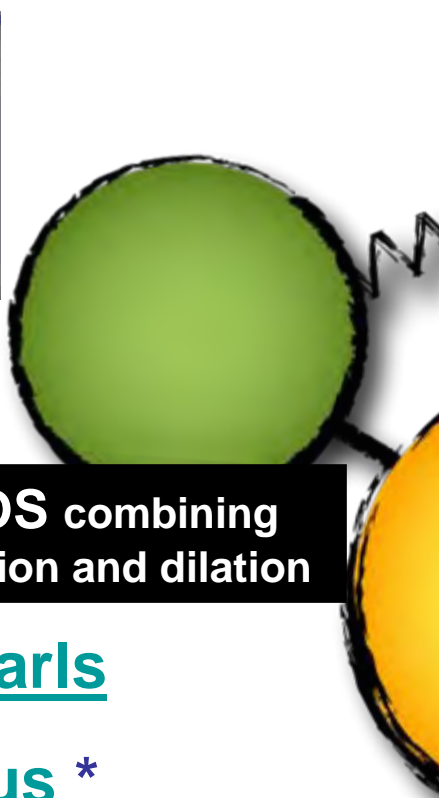
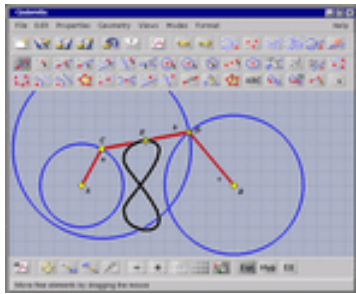
# Chaos Games in Genetics



# (Euclidean) Reflection in a Circle:



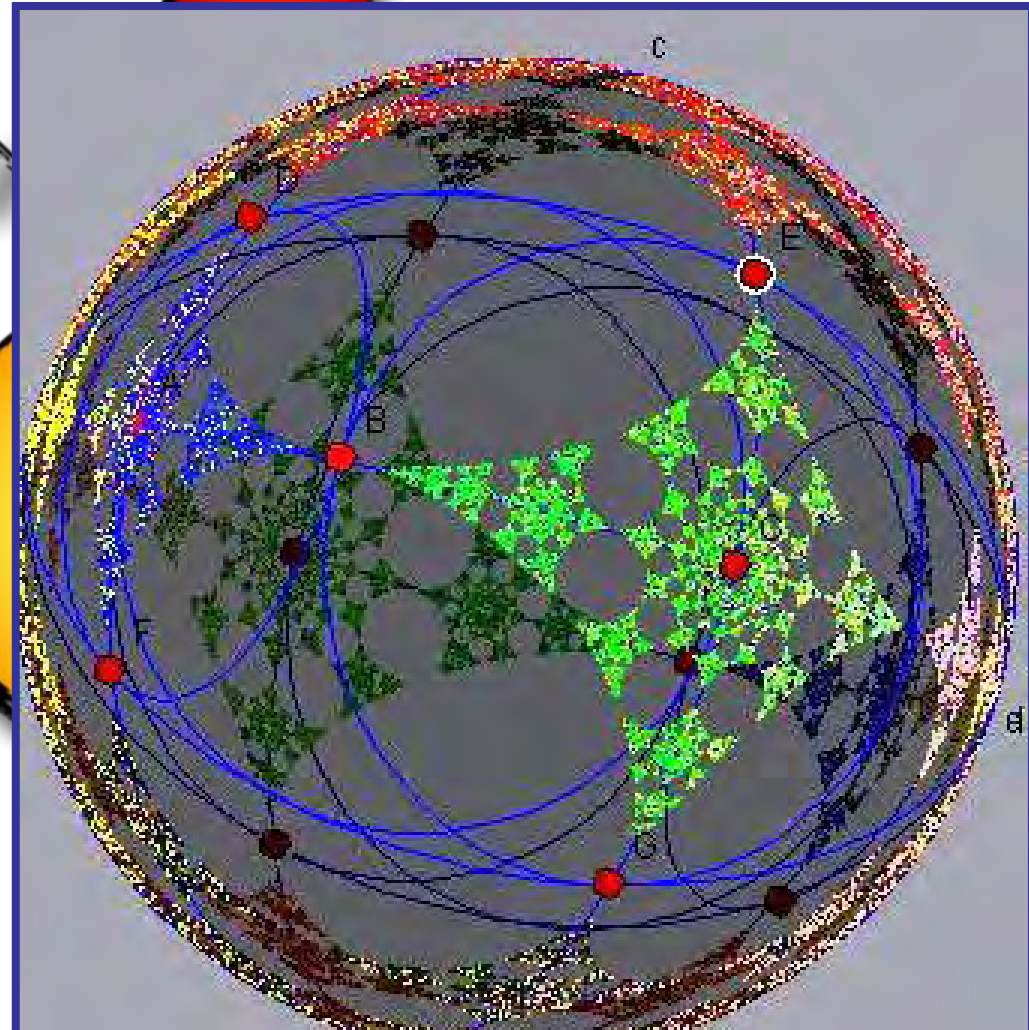
# CINDERELLA's dynamic geometry



[www.cinderella.de](http://www.cinderella.de)

**FOUR DEMOS** combining inversion, reflection and dilation

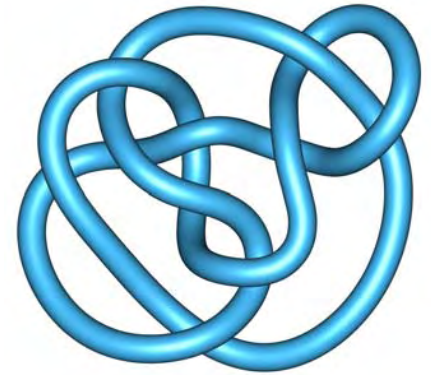
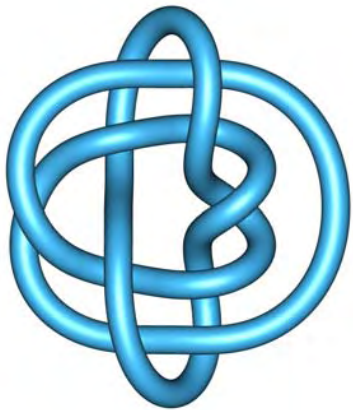
1. [Indraspearls](#)
2. [Apollonius](#) \*
3. [Hyperbolicity](#)
4. [Gasket](#)



# KnotPlot's Interactive Proofs

**The Perko Pair  $10_{161}$  and  $10_{162}$**

are two adjacent 10-crossing knots (1900)



First shown to be the same by Ken Perko in 1974  
and beautifully made dynamic in [KnotPlot](#) (open source)



# Outline. What is HIGH PERFORMANCE MATHEMATICS?

## 1. Visual Data Mining in Mathematics.

- ✓ Fractals, Polynomials, Continued Fractions\*
- ✓ Pseudospectra and Code Optimization



## 2. High Precision Mathematics.

## 3. Integer Relation Methods.

- ✓ Chaos, Zeta\* and the Riemann Hypothesis,
- ✓ Hex-Pi and Normality



## 4. Inverse Symbolic Computation.

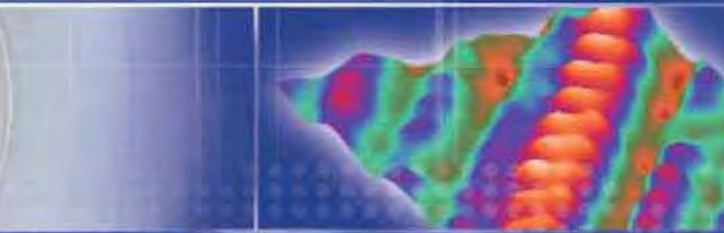
- ✓ A problem of Knuth\*,  $\pi/8$ , Extreme Quadrature

## 5. Conclusion.

# CONCLUSION

## ENGINES OF DISCOVERY: The 21st Century Revolution

The Long Range Plan for High Performance Computing in Canada



# The LRP tells a Story

- The Story
- Executive Summary
- Main Chapters
  - Technology
  - Operations
  - HQP
  - Budget

25 Case  
Studies  
– many  
sidebars

## One Day ...

**High-performance computing (HPC) affects the lives of Canadians every day. We can best explain this by telling you a story. It's about an ordinary family on an ordinary day, Russ, Susan, and Kerri Sheppard. They live on a farm 15 kilometres outside Wyoming, Ontario. The land first produced oil, and now it yields milk; and that's just fine locally.**

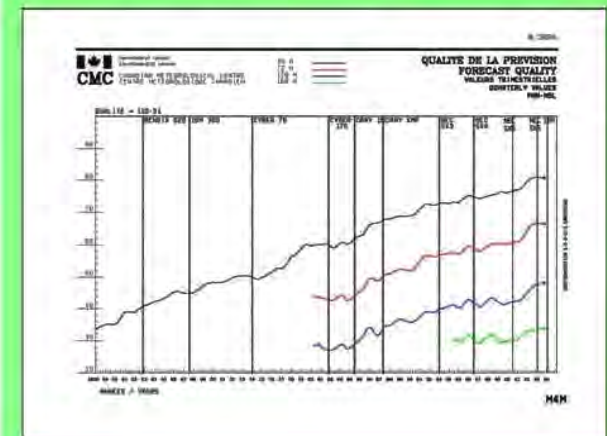
Their day, Thursday, May 29, 2003, begins at 4:30 am when the alarm goes off. A busy day, Susan Zhong-Sheppard will fly to Toronto to see her father, Wu Zhong, at Toronto General Hospital; he's very sick from a stroke. She takes a quick shower and packs a day bag for her 6 am flight from Sarnia's Chris Hadfield airport. Russ Sheppard will stay home at their dairy farm, but his day always starts early. Their young daughter Kerri can sleep three more hours until school.

Waiting, Russ looks outside and thinks, *It's been a dryish spring. Where's the rain?*

In their farmhouse kitchen on a family-sized table sits a PC with a high-speed Internet line. He logs on and finds the Farmer Daily site. He then chooses the Environment Canada link, clicks on Ontario, and then scans down for Sarnia-Lambton.

## WEATHER PREDICTION

The "quality" of a five-day forecast in the year 2003 was equivalent to that of a 36-hour forecast in 1963 [REF 1]. The quality of daily forecasts has risen sharply by roughly one day per decade of research and HPC progress. Accurate forecasts transform into billions of dollars saved annually in agriculture and in natural disasters. Using a model developed at Dalhousie University (Prof. Keith Thompson), the Meteorological Service of Canada has recently been able to predict coastal flooding in Atlantic Canada early enough for the residents to take preventative action.





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that makes so  
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