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



Dalhousie Distributed Research Institute and Virtual Environment



What is HIGH PERFORMANCE MATHEMATICS?

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

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





Revised 06/05/06



George Polya 1887-1987



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



Drive

How-To Training Sessions

Brought to you using Access Grid technology

For more information contact Jana at 210-5489 or 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

STORE.

A = = = 1

Ø 17



What is HIGH PERFORMANCE MATHEMATICS?

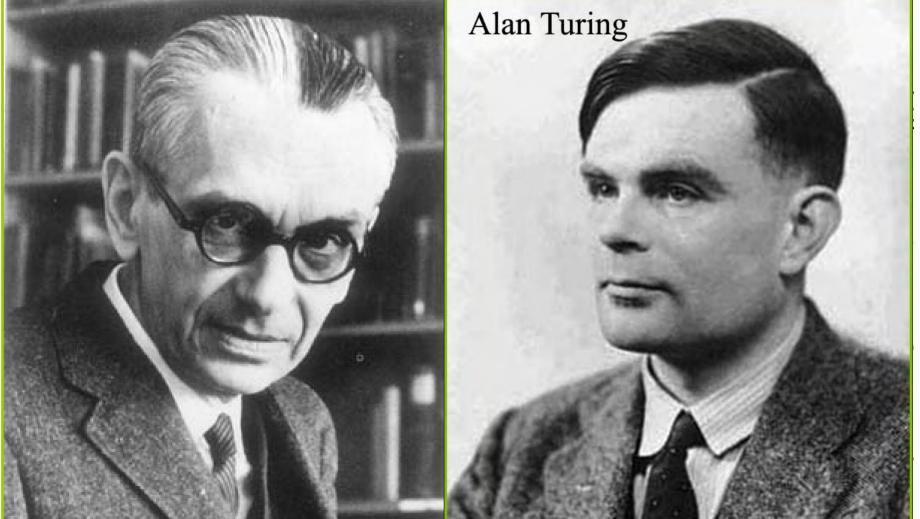


Dalhousie Distributed Research Institute and Virtual Environment

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

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)



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

From the Magazine | Innovators

Chaitin's universal halting constant

By MICHAEL D. LEMONICK

The Omega Man

It Doesn't Figure 111001100100111100010010011100 (Calude)

From the Sep. 12, 2005 issue Posted Sunday, Sep. 04, 2005 and Scientific American March 2006

Online Edition

Over the past few decades, G IBM's T.J. Watson Resea N.Y., has been uncovering higher math may be riddle really a collection of random reason. And rather than principles, "I'm making th like done more physics

experim I'm dead

Chaitin's idea complicated help make or math: Gödel' system of ma particular cor

Sounds mathematica night and wo



Pour voir comment la valeur du nombre Ω (oméga) est définie, voici un exemple simplifié. Supposons que l'ordinateur considéré n'ait que trois programmes qui s'arrêtent et qu'ils soient représentés par les chaînes de bits 110, 11100 et 11110. Ces programmes ont, respectivement, une longueur de 3, 5 et 5 bits. Si nous choisissons un programme par hasard en tirant à pile ou face chaque bit, la probabilité de trouver ces chaînes est respectivement de 1/2³, 1/2⁵ et 1/2⁵, la probabilité pour chaque bit étant 1/2. La valeur de Ω , la probabilité d'arrêt, pour cet ordinateur particulier, est donc donnée par :

 $\Omega = \frac{1}{2^3} + \frac{1}{2^5} + \frac{1}{2^5} = 0,001 + 0,00001 + 0,00001 = 0,00110$ (en écriture binaire). Ce nombre binaire correspond à la probabilité d'obtenir l'un des trois arrêts par hasard - c'est la probabilité que notre ordinateur s'arrêtera.

Comme le programme 110 s'arrête, nous ne considérons pas de programmes commençantpar 110 etplus longs, par exemple 1100 ou 1101. Par conséguent, il n'y a pas à ajouter des termes de type 0,0001 pour chacun de ces programmes. On considère tous les programmes tels que 1100 et ainsi de suite comme décrits par le programme qui s'achève 110. Quand ces programmes s'arrêtent, ils arrêtent de réclamer des bits supplémentaires.

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.
- **3. Integer Relation Methods.**
 - ✓ Chaos, Zeta* and the Riemann Hypothesis
 - ✓ Hex-Pi and Normality
- 4. Inverse Symbolic Computation.

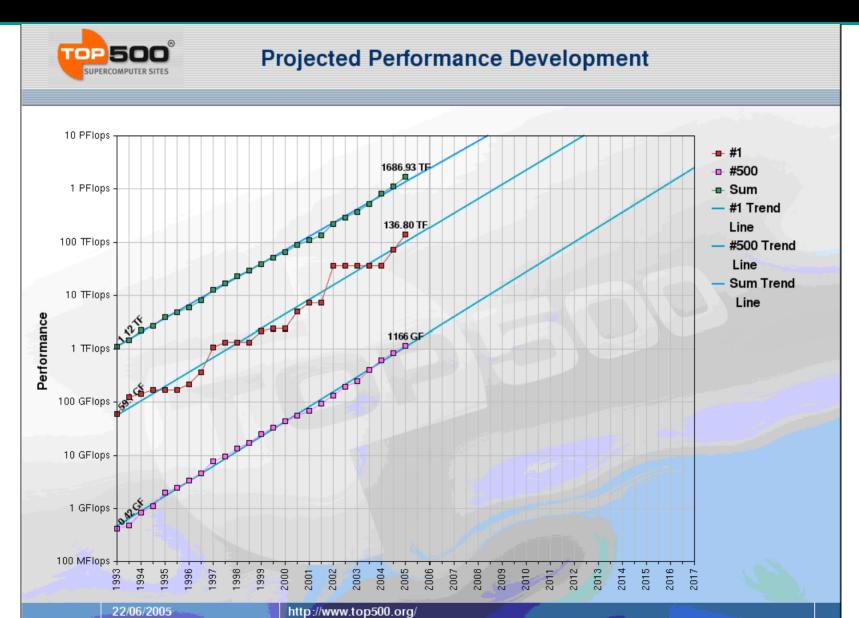
✓ A problem of Knuth*, π /8, Extreme Quadrature

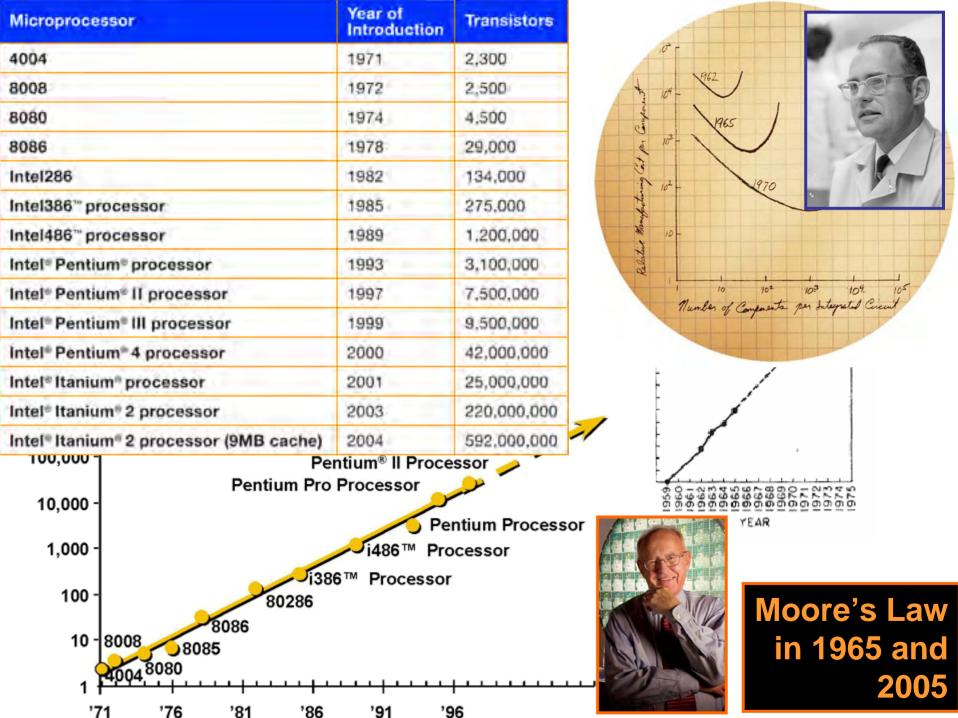
5. Demos and Conclusion.





Moore's 1965 Law continues:





This picture is worth 100,000 ENIACs

A. ..

The past

2 3 7

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

NERSC's 6000 cpu Seaborg in 2004 (10Tflops/sec) - we need new software paradigms for `bigga-scale' hardware



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



2¹⁷ 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 M

The reader who wants to get an introduction to this excitin approach to doing mathematics can do no better than the —Notices of t

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

This Experiments in Mathematics CD contains the full text of b matics by Experiment: Plausible Reasoning in the 21st Century a mentation in Mathematics: Computational Paths to Discovery i searchable form. The CD includes several "smart" enhancement

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

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

ISBN 1-5

EXPERIMENTS IN MATHEMATICS

Jonathan M. Borwein David H. Balley Roland Girgensohn Produced with the assistance of Mason Macklem 🗡 AK Peters, Ltd.

to read!... how to become atician." Scientist Online



A K Peters, Ltd.

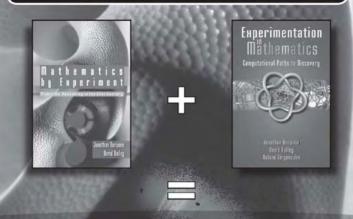
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AKPETERS

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



xperiments in Mathematics

han M. Borwein, David H. Bailey, Roland Girge

short time since the first editions of Mathematics by Experiment: Plausible Reason st Century and Experimentation in Mathematics: Computational Paths to Discovery een a noticeable upsurge in interest in using computers to do real mathematics. The updated and enhanced the book files and have now made them available in PDF form DM. 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

gmented search facility assists one with a search for particular mathematical form ssions. These enhancements will significantly improve the usability of these files and tself will enhance the reader's experience.



Coming Coning 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



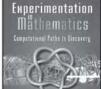
"... experimental mathematics is here to stay. The reader who wants to get an introduction to this exciting approach to doing mathematics can do no better than [this book]."

- 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 humanand 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 Mathodology

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

MATH LAB

Computer experiments are transforming mathematics

BY ERICA KLARREICH

Science News 2004

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 mathcomatician at Reed College in Portland, Ore. "Instead of just being a number-erunching tool, the computer is becoming more like a garden abovel that turns over rocks, and you find things underneath."

At the same time, the new work simp 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, "Borvein asys. "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.

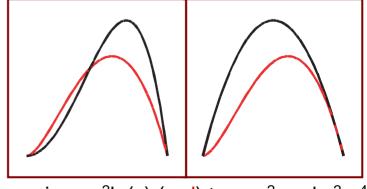
For instance, in 1666, sheer curiosity and love of numbers led Isaac Newton to calculate directly the first 16 digits of the number pi, later writing, "I am ashamed to tell you to how many figures I carried these computations, having no other business at the time." Carl Friedrich Gauss, one of the towering figures of 19th-cen-

tury mathematics, habitually discovered new mathematical results by experimenting with numbers and looking for patterns. When Gauss was a teenager, for instance, his experiments led hin 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 xdivided by the locarithm of x.

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

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

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



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

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 !

 \diamond For n = 3 this is

6 TERMS LIKE

 $q_1 q_2 q_3 (\frac{1}{q_1 + q_2 + q_3}) (\frac{1}{q_2 + q_3}) (\frac{1}{q_3})$

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

• 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 $N \in \mathbb{N}$

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

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.]

Also in ToVA -- find a direct proof?

Convex integrand

True, but why?

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

The candidates:

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

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

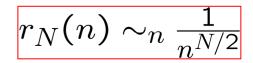
$$\frac{128}{\pi^2} = \sum_{n=0}^{\infty} r_5(n) \left(820n^2 + 180n + 13\right) \left(\frac{-1}{4^5}\right)^n$$

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

Here, in terms of factorials and rising factorials:

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

The 4th is only true



S.Ramanujan 1887-1920

Grand Challenges in Mathematics (CISE 2000)

are few and far between

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



Fano plane of

order 2

On an upcoming slide

- Nonexistence of Projective Plane of Order 10
 - 10²+10+1 lines and points on each other (n+1 fold)
 - 2000 Cray hrs in 1990
 - next similar case:18 needs10¹² hours?
 - or a Quantum Computer

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



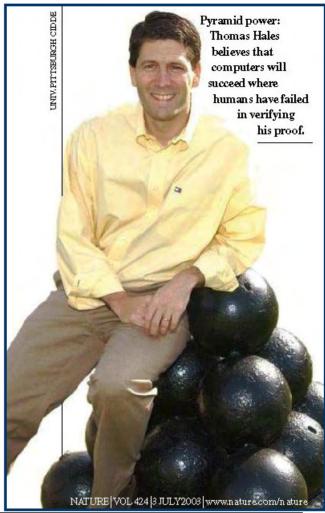
Cultural Maps in Mathematics

"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."

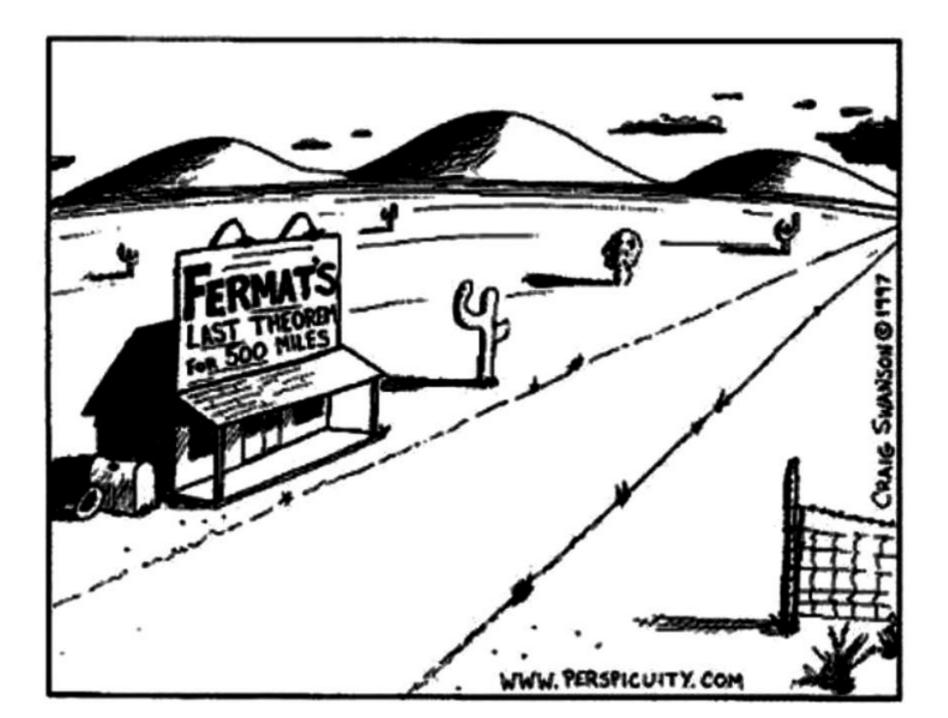
(Johann Wolfgang von Goethe) Maximen und Reflexionen, no. 1279

- 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





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



Coast to Coast Seminar Series



Tuesdays 3:30 – 4:30 pm Atlantic Time

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

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



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

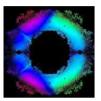


Shared Desktop for viewing presentations or sharing software

The AG in Action

in CoLab





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

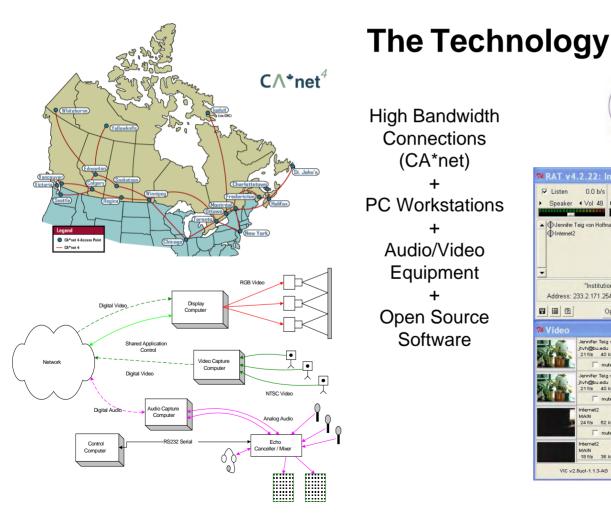




Karl Dilcher, Dalhousie University

Fermat Numbers, Wieferich and Wilson Primes



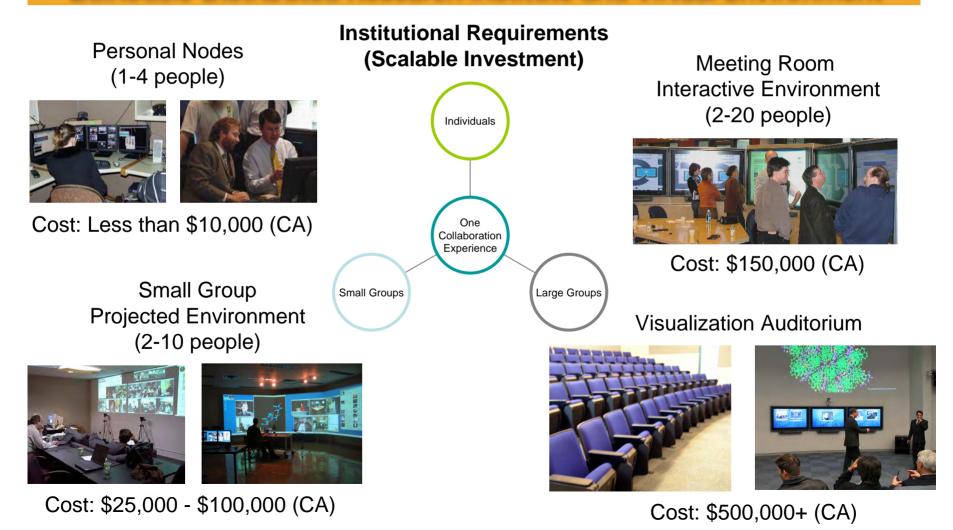


High Bandwidth Connections (CA*net) PC Workstations Audio/Video Equipment **Open Source** Software









Six degrees of net separation ...

5 Smart Shared-Screens







Being emulated by the Canadian Kandahar mission

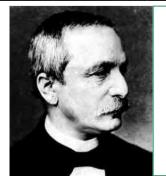
I shall now show a variety of uses of high performance computing and communicating as part of

Experimental Inductive Mathematics

Our web site:

www.experimentalmath.info

contains all links and references



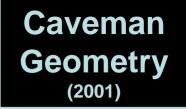
AMS Notices

Cover Article

Drive

"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



Very cool for the one person with control

The 2,500 sq-metre IRMACS research centre



SFU building is a also a 190cpu G5 Grid

At the official April opening, I gave one of the four presentations from D-DRIVE



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

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- 4. Inverse Symbolic Computation.
 - ✓ A problem of Knuth*, π /8, Extreme Quadrature
- 5. Demos and Conclusion.





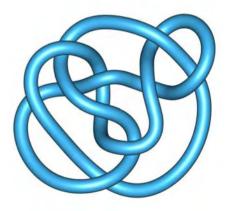
Interactive Proofs

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 <u>KnotPlot</u> (open source)

More Mathematical Data Mining

Experimentation

Mathematics

Computational Paths to Discovery

athematics HEHPERIMENT

Jonathan Borwein

Bavid Bailey

An unusual Mandelbrot parameterization

Various visual examples follow

- Indra's pearls
- Roots of `1/-1' polynomials
- Ramanujan's fraction
- **Sparsity and Pseudospectra**

AK Peters, 2004 (CD in press)

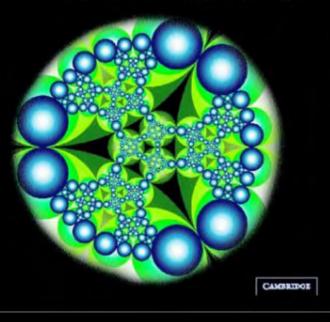
n Barwein

Roland Birgensohn

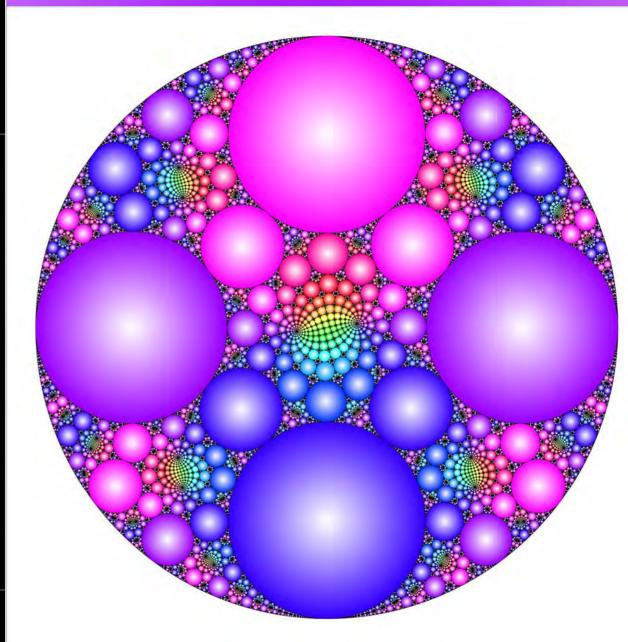
ໄກປາຍ'ອ Pອຍປອ A merging of 19th and 21st Centuries

INDRA'S PEARLS The Vision of Felix Klein

David Mumford, Caroline Series, David Wright



Double cusp group

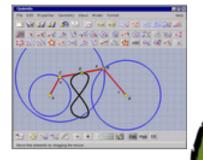


2002: http://klein.math.okstate.edu/IndrasPearls/



CINDERELLA's dynamic geometry

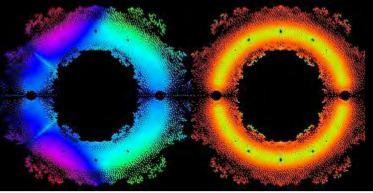






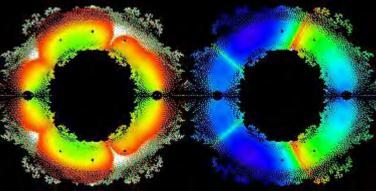


- 1. Indraspearls
- 2. Apollonius *
- 3. Hyperbolicity
- 4. Gasket



Roots of Zeros

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



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

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

- <u>All</u> zeros are pictured (at **3600 dpi**)
- Figure 1b is colored by their local density
- Figure 1d shows sensitivity relative to the x⁹ term
- The white and orange striations are not understood

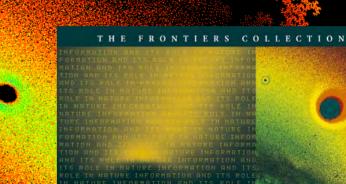
A wide variety of patterns and features become visible, leading researchers to totally unexpected mathematical results

"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, <u>Interview</u>, 2000.

The TIFF on VARIOUS SCALES

Pictures are more democratic but they come from formulae

Roots in the most stable colouring



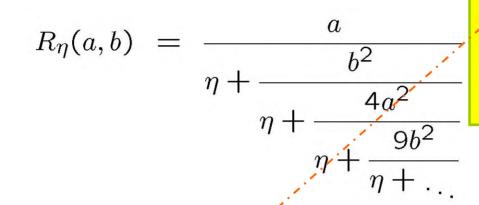
J. G. Roederer







Ramanujan's Arithmetic-Geometric Continued fraction (CF)



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

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

Cardiod

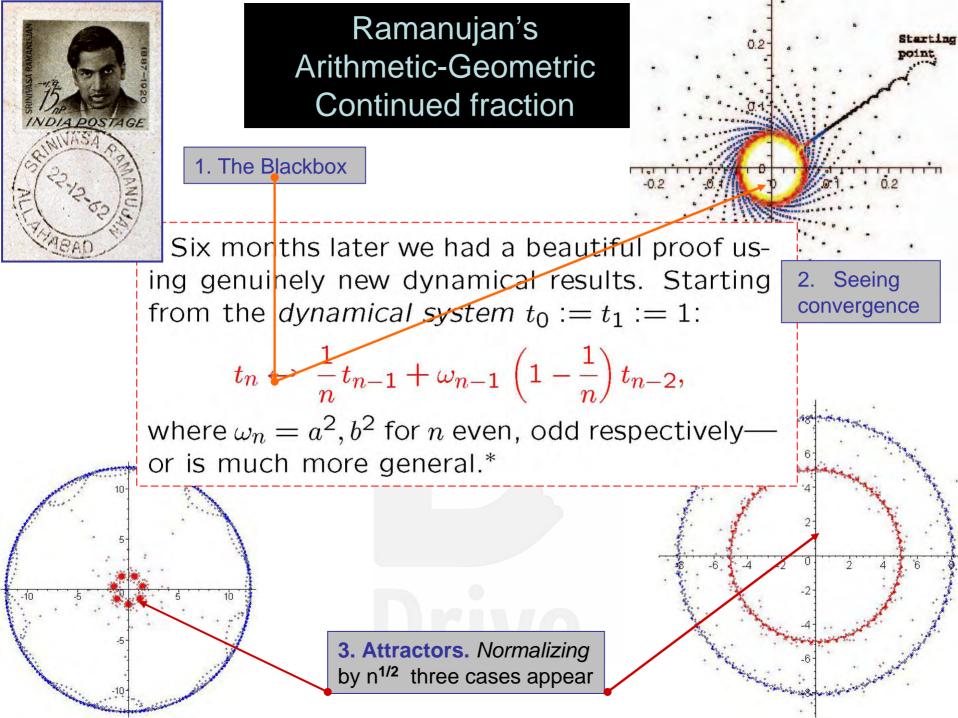
 $|\frac{a+b}{a+b}|$

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

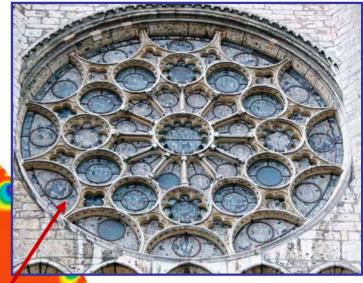
We wished to know for which a/b in C this all held

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

Which discovery it remained to prove?



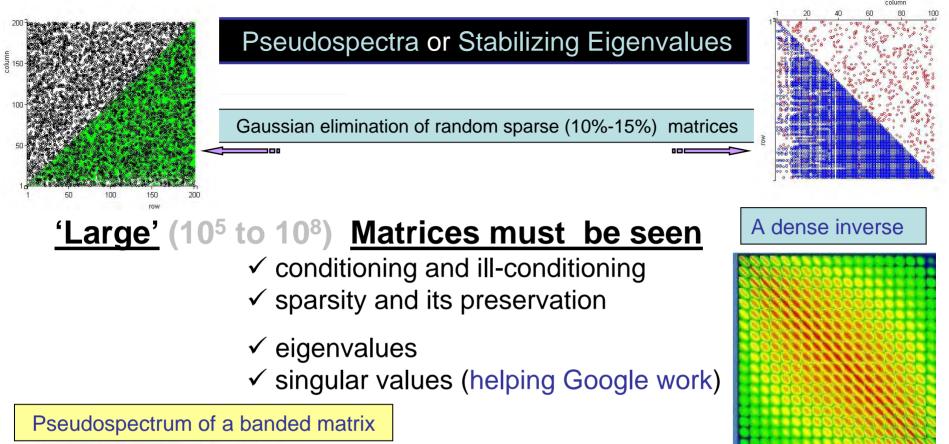
Mathematics and the aesthetic Modern approaches to an ancient affinity (CMS-Springer, 2005)

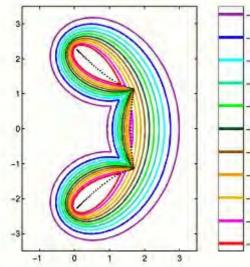


Why should I refuse a good dinner simply because I don't understand the digestive processes involved?

> Oliver Heaviside (1850 - 1925)

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



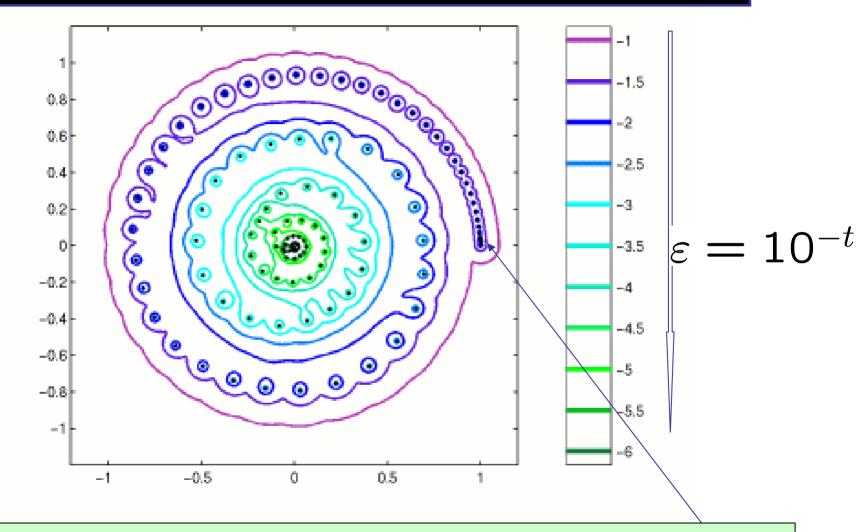


The pseudo spectrum of A: for $\varepsilon > 0$

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

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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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 α is algebraic of degree d and length λ (coefficient sum in absolute value)

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

Example (MAA, April 2005). Prove that

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

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

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

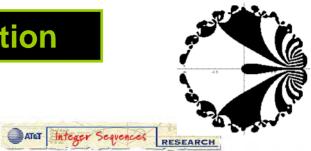
Numeric and Symbolic Computation

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

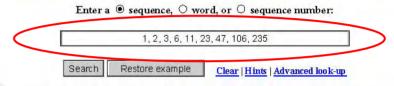
- ✓ Massive (serial) Symbolic Computation
 - Automatic differentiation code
- ✓ Integer Relation Methods

Inverse Symbolic Computation





The On-Line Encyclopedia of Integer Sequences



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

For information about the Encyclopedia see the Welcome page

Lookup | Welcome | Francais | Demos | Index | Browse | More | Web Cam Contribute new seq. or comment | Format | Transforms | Puzzles | Hot | Classics More pages | Superseeker | Maintained by N. J. A. Sloane (njas@research.att.com)

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

Other useful tools : Parallel Maple

- Sloane's online sequence database
- Salvy and Zimmerman's generating function package 'gfun'

 Automatic identity proving: Wilf-Zeilberger method for hypergeometric functions

Greetings from the On-Line Encyclopedia of Integer Sequences!



Matches (up to a limit of 30) found for 1 2 3 6 11 23 47 106 235 : [It may take a few minutes to search the whole database, depending on how many matches are found (the second and later look are faster)]

An Exemplary Database

 ID Number:
 A000055
 (Formerly M0791 and N0299)

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

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

5469566585,14830871802,40330829030,109972410221

Name: Number of trees with n unlabeled nodes.

- Comments: Also, number of unlabeled 2-gonal 2-trees with n 2-gons.
- References F. Bergeron, G. Labelle and P. Leroux, Combinatorial Species and Tree-Like Structures, Camb. 1998, p. 279.
 - N. L. Biggs et al., Graph Theory 1736-1936, Oxford, 1976, p. 49.
 - S. R. Finch, Mathematical Constants, Cambridge, 2003, pp. 295-316.
 - D. D. Grant, The stability index of graphs, pp. 29-52 of Combinatorial Mathematics (Proceedings 2nd Australian Conf.), Lect. Notes Math. 403, 1974.
 - F. Harary, Graph Theory. Addison-Wesley, Reading, MA, 1969, p. 232.
 - F. Harary and E. M. Palmer, Graphical Enumeration, Academic Press, NY, 1973, p. 58 and 244.
 - D. E. Knuth, Fundamental Algorithms, 3d Ed. 1997, pp. 386-88.
 - R. C. Read and R. J. Milson, An Atlas of Graphs, Oxford, 1998.
 - J. Riordan, An Introduction to Combinatorial Analysis, Wiley, 1958, p. 138.
- Links: P. J. Cameron, <u>Sequences realized by oligomorphic permutation groups</u> J. Integ. Seqs. Vo Steven Finch, <u>Otter's Tree Enumeration Constants</u>
 - 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. M. Weisstein, Link to a section of The World of Mathematics.

Index entries for sequences related to trees

Index entries for "core" sequences

G. Labelle, C. Lamathe and P. Leroux, Labeled and unlabeled enumeration of k-gonal 2-tr

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





Integrated real time use

- moderated

- 120,000 entries

- grows daily

- AP book had 5,000



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 <u>other operations</u>

via Newton's method

$$\times,\div,\sqrt{\cdot}$$

• Elementary and special functions via Elliptic integrals and Gauss AGM $O(n^{\log_2(3)})$

For example:

Karatsuba replaces one 'times' by many 'plus'

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

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:

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

 $C_4 = 14\zeta(3)$ lim $C_n = 2e^{-2\gamma}$

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

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

- 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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Integer Relation Methods

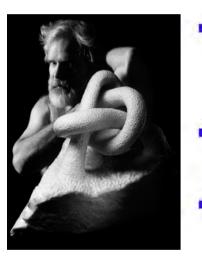
The PSLQ Integer Relation Algorithm





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

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



- 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 x n digits, where d is the size (in digits) of the largest of the integers a_k .

An Immediate Use

To see if a is algebraic of degree N, consider (1,a,a²,...,a^N)

Combinatorial optimization for pure mathematics (also LLL)

Application of PSLQ: Bifurcation Points in Chaos Theory



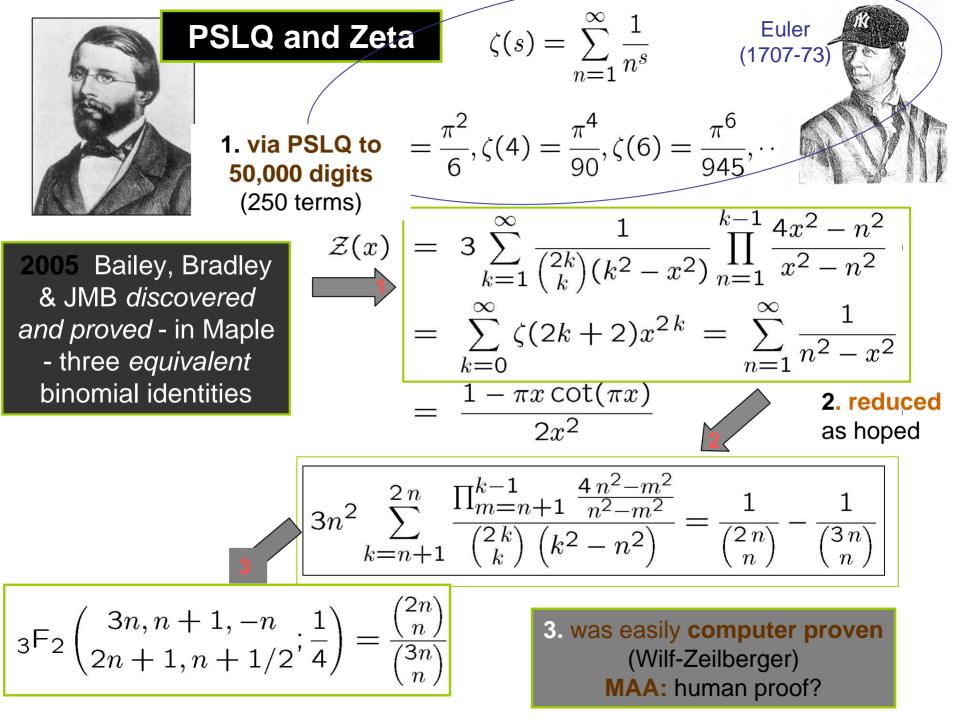
B₃ = 3.54409035955... is third bifurcation point of the logistic iteration of chaos theory:

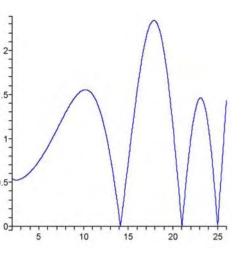
 $x_{n+1} = rx_n(1-x_n)$

- i.e., B₃ is the smallest r such that the iteration exhibits 8way periodicity instead of 4-way periodicity.
- In 1990, a predecessor to PSLQ found that $\rm B_3$ 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 B₄ 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





The imaginary parts of first 4 zeroes are:

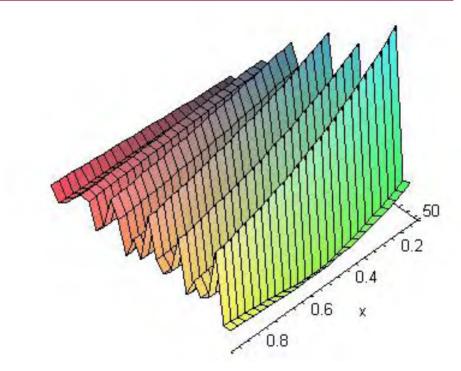
14.134725142 21.022039639

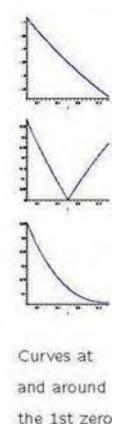
25.010857580 30.424876126

The first 1.5 billion are on the *critical line*

Yet at 10²² the "*Law of small numbers*" still rules (Odlyzko)

Visualizing the Riemann Hypothesis (A Millennium Problem)

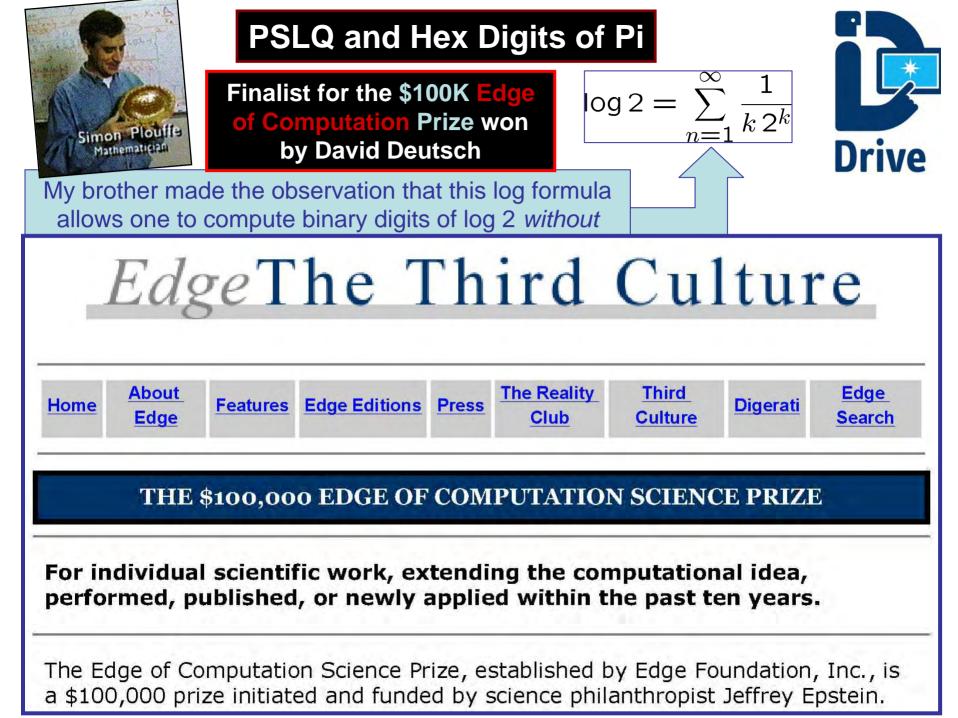




.....

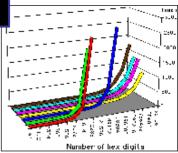
'All non-real zeros have real part one-half' (The Riemann Hypothesis)

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



The pre-designed Algorithm ran the next day

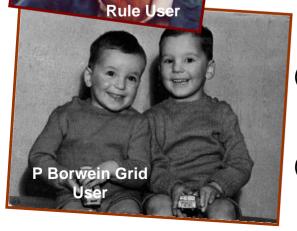
ALGORITHMIC PROPERTIES



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

Now built into some compilers!

- (2) is implementable on any modern computer;
- (3) requires no multiple precision software;



D Borwein Slide

J Borwein

Abacus User and Computer Racer

(4) requires very little memory; and



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

000	PiHex- A distributed effort to calculate Pi		
🔶 🄶 🚽 🔶	http://www.cecm.sfu.ca/	/projects/pihex/	▼ © (<u>G</u> •
Getting Started Latest Headline	es 就 www.icbc.ca		
PiHex ha	The I The	e Quadrillionth Bit of P Forty Trillionth Bit of Five Trillionth Bit of I	Pi is '0'!
hits since the counter last reset.	Position	Hex Digits Beginnin At This Positio	
Undergraduate Colin Percival's grid computation PiHex rivaled Finding Nemo	$ \begin{array}{c} 10^{6} \\ 10^{7} \\ 10^{8} \\ 10^{9} \\ 10^{10} \\ 10^{11} \\ 1.25 \times 10^{12} \end{array} $	26C65E52CB45 17AF5863EFED ECB840E21926 85895585A042 921C73C6838F 9C381872D275 07E45733CC79	$\begin{array}{c c} & & & & & & & \\ & & & & & & \\ & & & & $
	2.5×10^{14}	E6216B069CB6	

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 GALILEOS TIME

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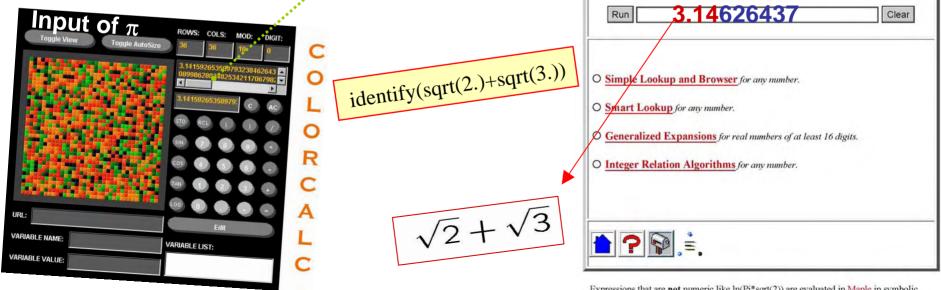
A Colour and an Inverse Calculator (1995)

Inverse Symbolic Computation

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

Inferring mathematical structure from numerical data

- Mixes large table lookup, integer relation methods and intelligent preprocessing — needs micro-parallelism
- It faces the "curse of exponentiality"
- Implemented as Recognize in Mathematica and identify in Maple
 Please enter a number or a Maple expression:



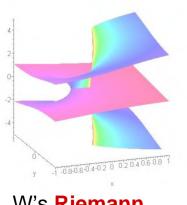
Expressions that are **not** numeric like ln(Pi*sqrt(2)) are evaluated in <u>Maple</u> in symbolic form first, followed by a floating point evaluation followed by a lookup.

Knuth's Problem

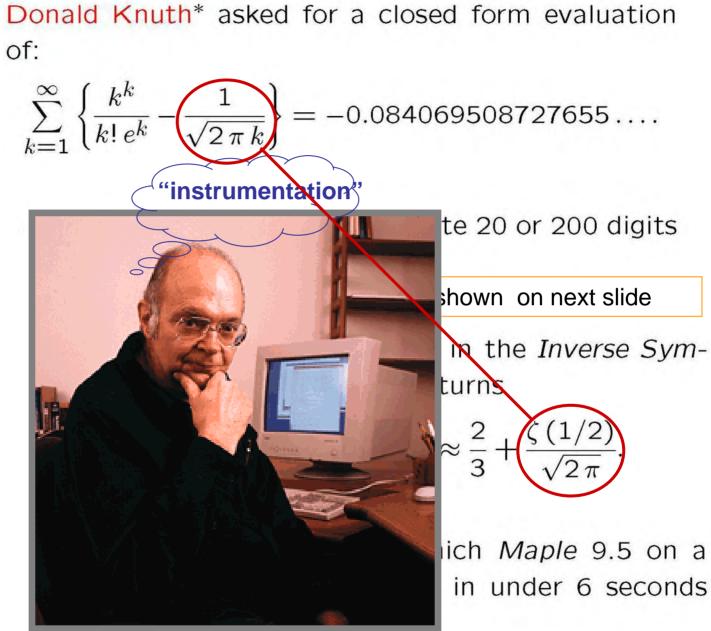
A guided proof followed on **asking why** Maple could compute the answer so fast.

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

 $W \exp(W) = x$



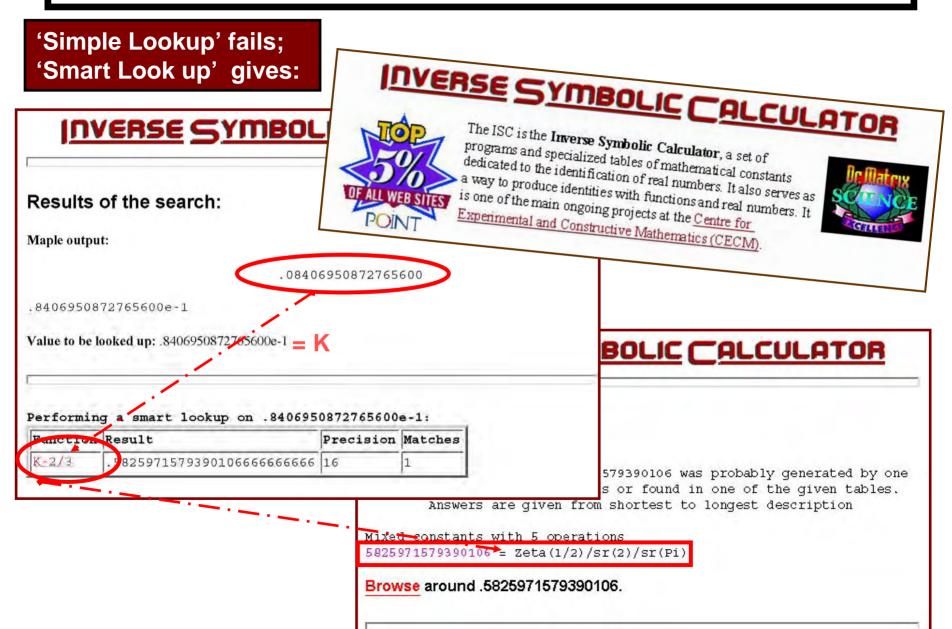
W's **Riemann** surface



* ARGUABLY WE ARE DONE

ENTERING

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



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.

We have certain

knowledge without

proof

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

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

- Ш. The integral was split at the nasty interior singularity Ш. The sum was `easy'.
- Ш. 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
 ✓ D₄ is a remarkable 1997 result due to McCoy--Tracy--Wu



An Extreme Ising Quadrature

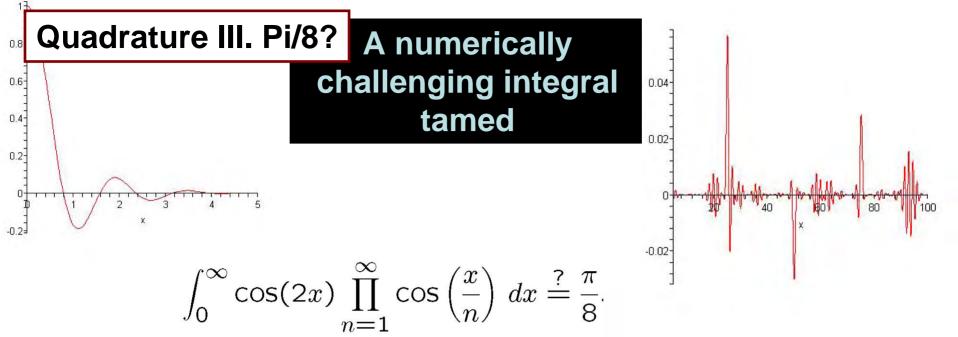
006 Recently Tracy asked for help 'experimentally' evaluating D₅

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...



Now $\pi/8$ equals

<u>0.39269908169872415480783042290993786052464</u>5434

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



Environment

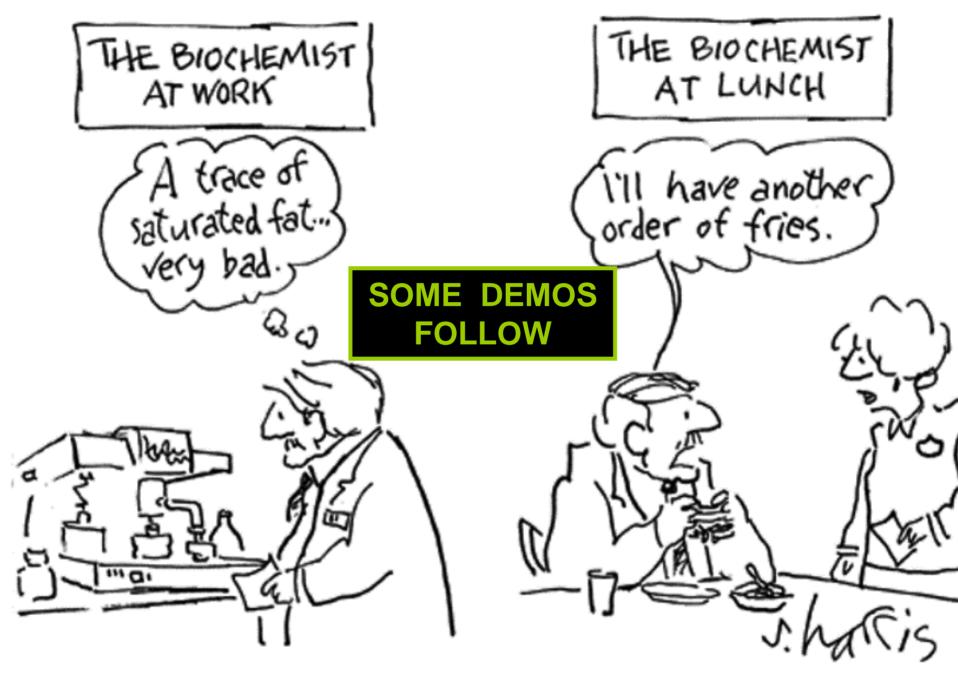
ics by Experiment: A.K. Peters, 2003.

ohn, *tational Paths to* Active CDs 2006]

ntal Mathematics: o*tices 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.



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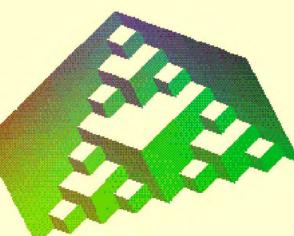
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Inverse Systems and Self-Similarity everywhere

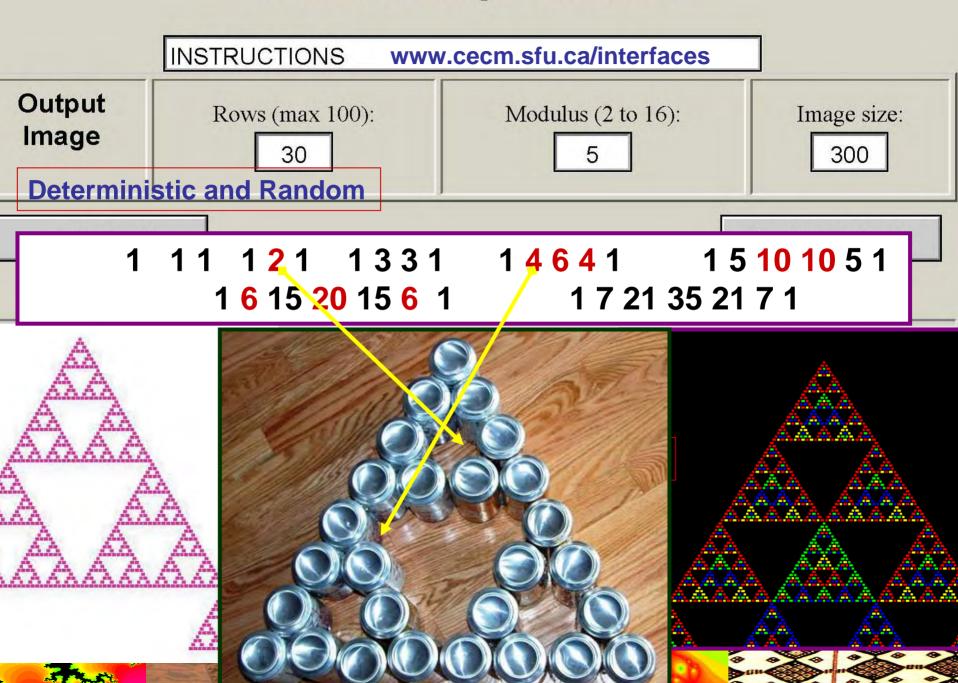
From Pascal and Sierpinski to Julia, Fatou & Mandelbrot



'cut and fold'

Truly modern mathematics in nature, art and applications

Pascal's Triangle Interface





FRACTALINA



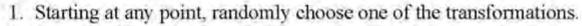
About Fractalina

Fractalina allows the input and itera play "the chaos game".

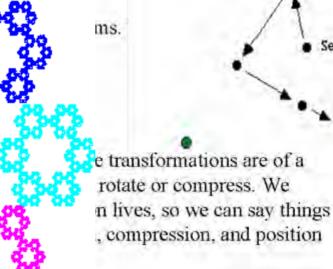
To see it in action, you can go direc

The chaos game begins with the sel special kind. Each transformation h sometimes informally think of the p like "go halfway to the transformati values that determine how it works.

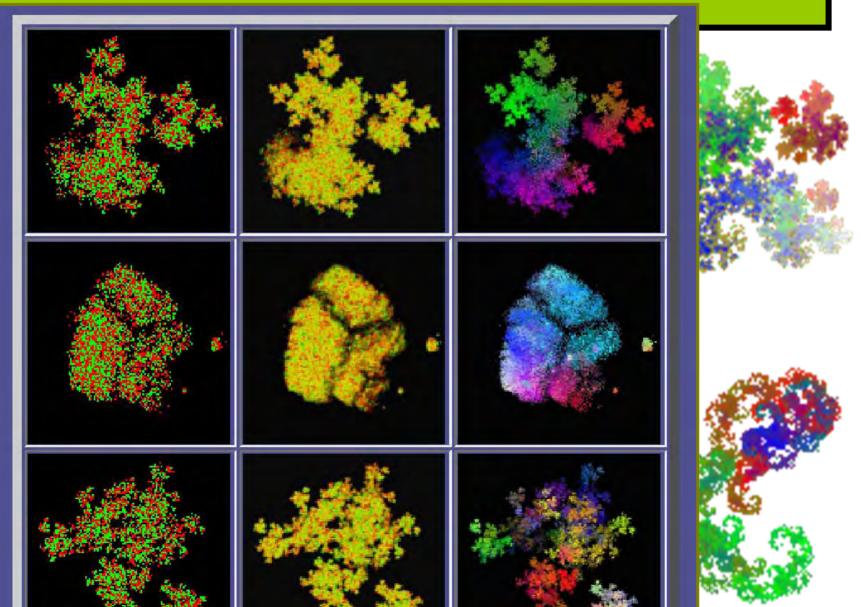
The chaos game can be explained this way:



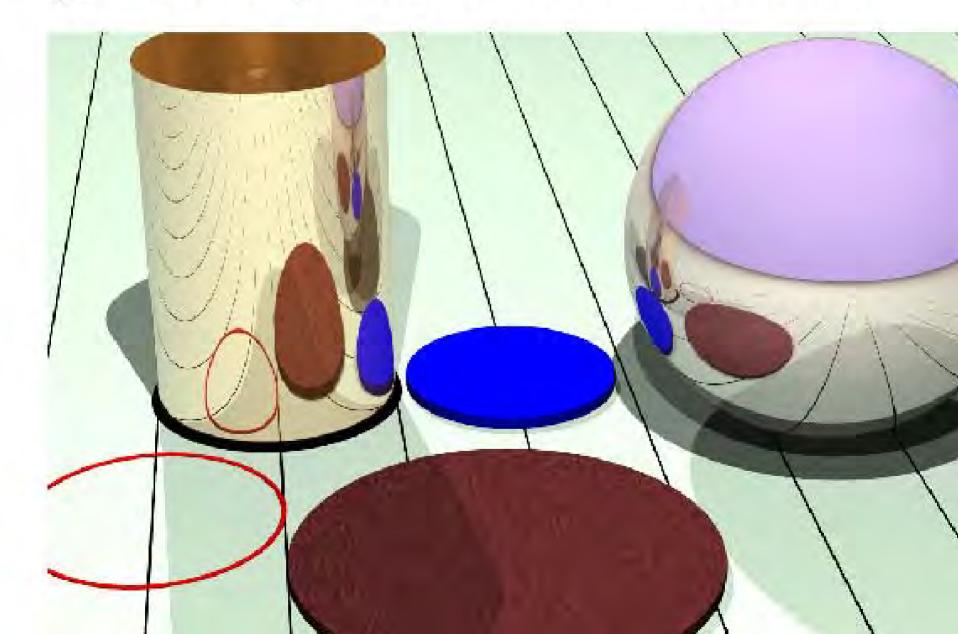
- 2. Go part of the way towards the center point of that transformation and rotate part way around it.
- 3. Repeat the process from the resulting point.



Chaos Games in Genetics



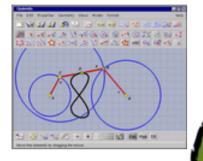
(Euclidean) Reflection in a Circle:





CINDERELLA's dynamic geometry







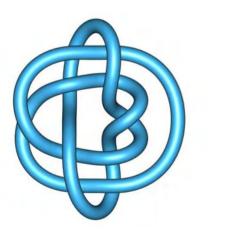


- 1. Indraspearls
- 2. Apollonius *
- 3. Hyperbolicity
- 4. Gasket

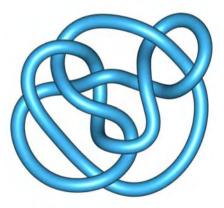
KnotPlot's Interactive Proofs

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 <u>KnotPlot</u> (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*, π /8, Extreme Quadrature

5. 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 – HOP

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.

