Second Annual

ONTARIO R&E SUMMIT

JUNE 13 & 14, 2005, COURTYARD BY MARRIOTT, DOWNTOWN TORONTO

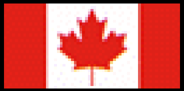
"Powering Ontario's Research Advantage"

orion

Drive

Dalhousie Distributed Research Institute and Virtual Environment

What is HIGH PERFORMANCE (Pure) MATHEMATICS?



Jonathan Borwein, FRSC www.cs.dal.ca/~jborwein

Canada Research Chair in Collaborative Technology

> *"I feel so strongly about the wrongness of reading a lecture that my language may seem immoderate .... The spoken word and the written word are quite different arts .... I feel that to collect an audience and then read one's material is like inviting a friend to go for a walk and asking him not to mind if you go alongside him in your car."*
>
> Sir Lawrence Bragg What would he say about Ppt?

Atlantic Computational Excellence Network

ACEnet

DALHOUSIE UNIVERSITY

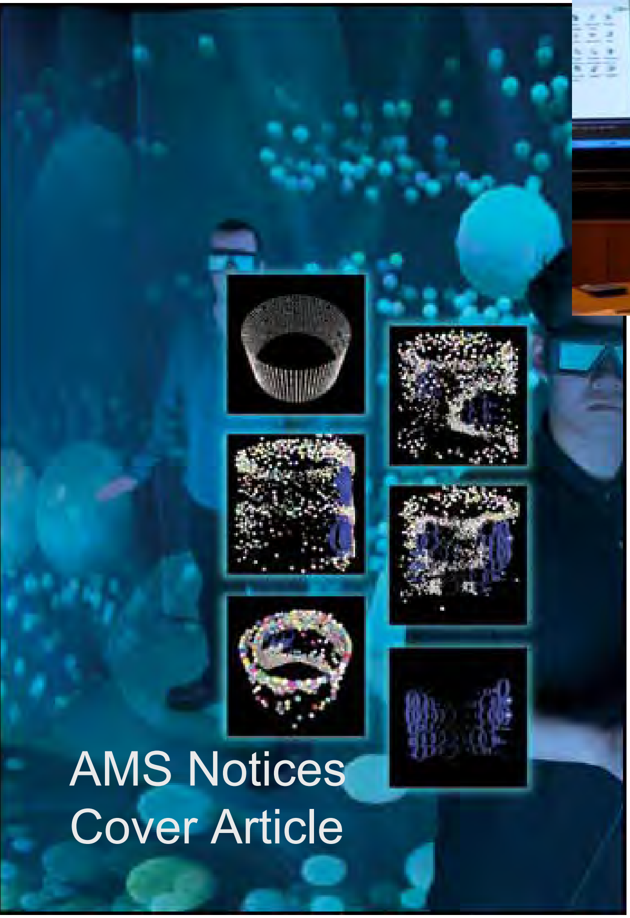
Inspiring Minds

Revised 14/06/05

WestGrid

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

5 SMART Touch-sensitive Interwoven Screens



AMS Notices
Cover Article

My intention is to show a variety of mathematical uses of high performance computing and communicating as part of

Experimental Inductive Mathematics

Our web site:

www.experimentalmath.info

contains all links and references

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

Harold Edwards, *Essays in Constructive Mathematics*, 2004

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
- Math and Science
  - Educational
  - Research

The 2,500 square metre IRMACS research centre

- ✓The building is a also a 190cpu G5 Grid
- ✓At the official April opening, I gave one of the four presentations from D-DRIVE

Trans-Canada Seminar Thursdays
PST 11.30 MST 12.30 AST 3.30

Centre seen as 'serious nirvana'

April 07, 2005 , vol. 32, no. 7

By Carol Thorbes

Move over creators of Max Head-room, Matrix and Metropolis. What researchers can accomplish at Simon Fraser University's IRMACS centre rivals the high tech feats of the most memorable futuristic films.

SFU mathematician and IRMACS executive director Peter Borwein (left) communicates with IRMACS collaboration and visualization coordinator Brian Corrie. To the right of them another plasma display portrays a 3D image of a molecular structure.

The $14 million centre's acronym stands for interdisciplinary research in the mathematical and computational sciences. The centre's expansive view of the

from atop

ain echoes its

al as a facility

tering

research

s whose

is the computer.

cted 2,500 square metre space atop the applied sciences building, the centre has eight

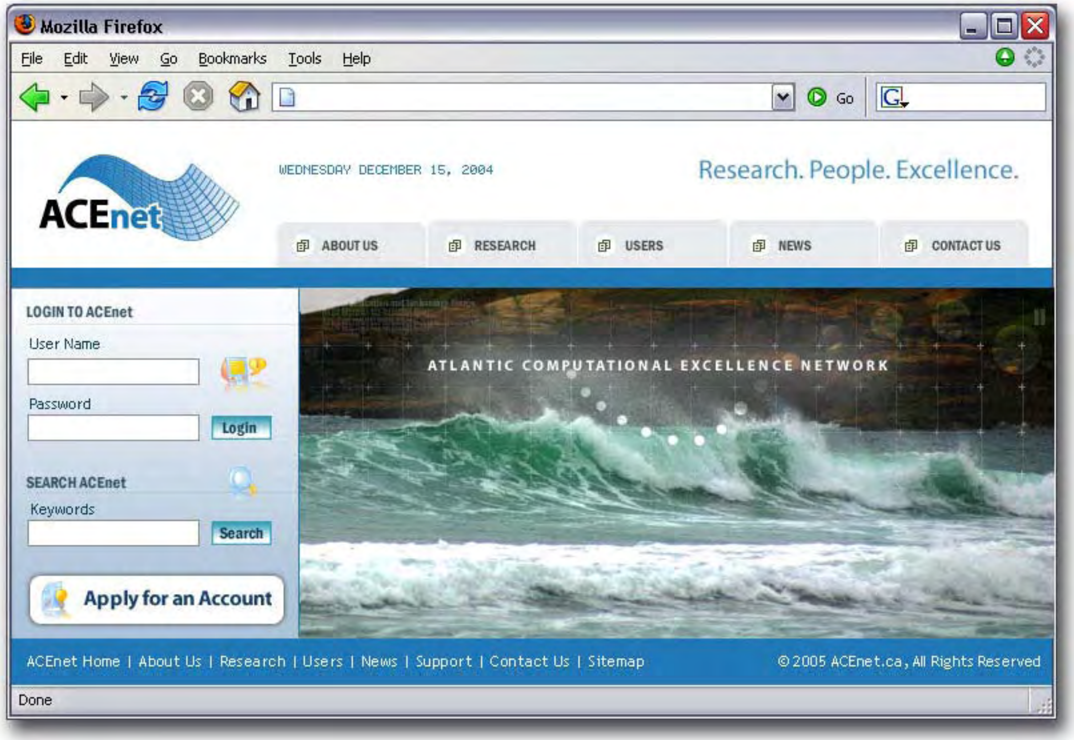
ng rooms and a presentation theatre, seating up to 100 people. They are equipped with

ble computational, multimedia, internet and remote conferencing (including satellite) technology. High performance distributed computing and clustering technology, designed at SFU, and access to WestGrid, an ultra high speed, interprovincial network, with shared computing and multimedia

The present

The AG in Action in CoLab

ACEnet to WestGrid



WEDNESDAY DECEMBER 15, 2004

Research. People. Excellence.

© 2005 ACEnet.ca, All Rights Reserved

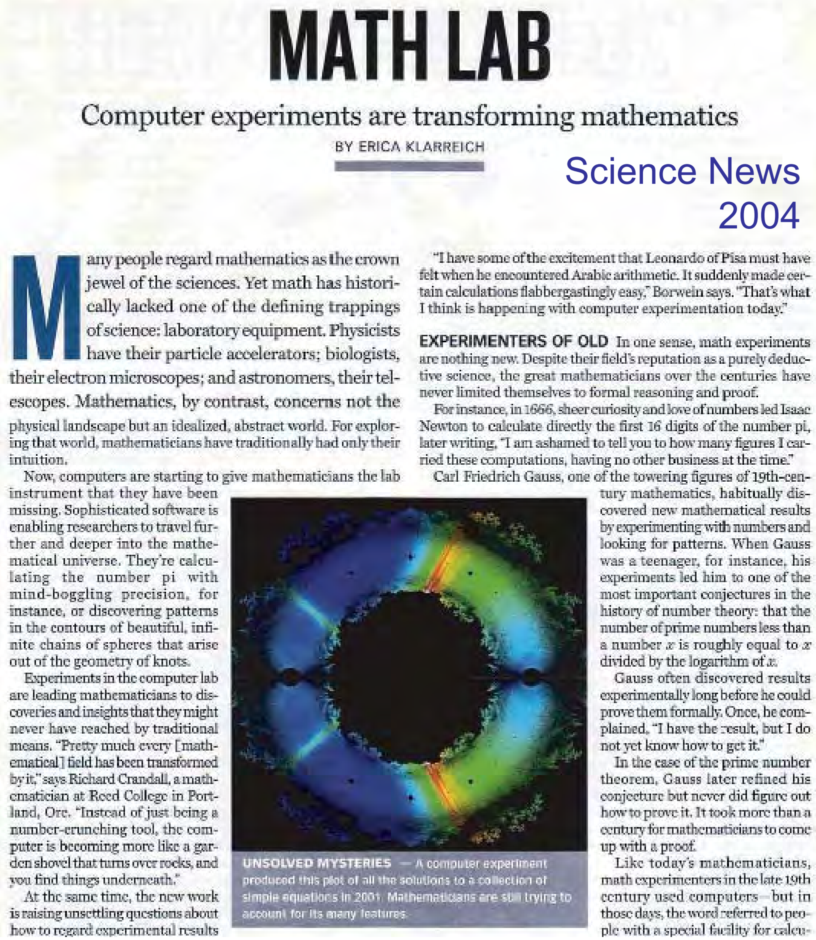
ACEnet completes the Pan Canadian Consortia

Enabling Canadian research excellence through high performance computing

Dalhousie's role will be in collaboration, visualization, and large data-set storage

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

Many people regard mathematics as the crown jewel of the sciences. Yet math has historically lacked one of the defining trappings of science: laboratory equipment. Physicists have their particle accelerators; biologists, their electron microscopes; and astronomers, their telescopes. Mathematics, by contrast, concerns not the physical landscape but an idealized, abstract world. For exploring that world, mathematicians have traditionally had only their intuition.

Now, computers are starting to give mathematicians the lab instrument that they have been missing. Sophisticated software is enabling researchers to travel further and deeper into the mathematical universe. They're calculating the number pi with mind-boggling precision, for instance, or discovering patterns in the contours of beautiful, infinite chains of spheres that arise out of the geometry of knots.

Experiments in the computer lab are leading mathematicians to discoveries and insights that they might never have reached by traditional means. "Pretty much every [mathematical] field has been transformed by it," says Richard Crandall, a mathematician at Reed College in Portland, Ore. "Instead of just being a number-crunching tool, the computer is becoming more like a garden shovel that turns over rocks, and you find things underneath."

At the same time, the new work is raising unsettling questions about how to regard experimental results

UNSOLVED MYSTERIES — A computer experiment produced this plot of all the solutions to a collection of simple equations in 2001. Mathematicians are still trying to account for its many features.

"I have some of the excitement that Leonardo of Pisa must have felt when he encountered Arabic arithmetic. It suddenly made certain calculations flabbergastingly easy," Borwein says. "That's what I think is happening with computer experimentation today."

EXPERIMENTERS OF OLD In one sense, math experiments are nothing new. Despite their field's reputation as a purely deductive science, the great mathematicians over the centuries have never limited themselves to formal reasoning and proof.

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

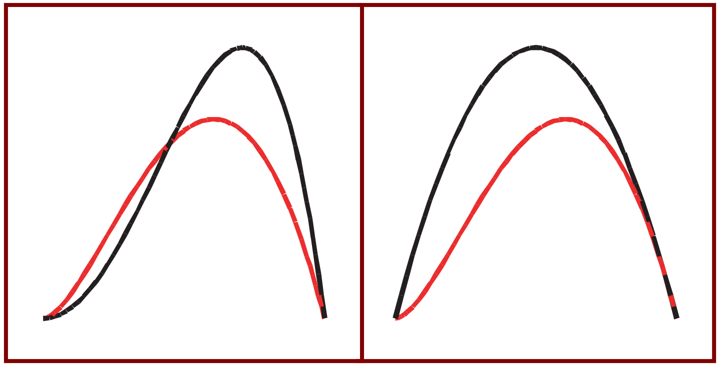
Carl Friedrich Gauss, one of the towering figures of 19th-century mathematics, habitually discovered new mathematical results by experimenting with numbers and looking for patterns. When Gauss was a teenager, for instance, his experiments led him to one of the most important conjectures in the history of number theory: that the number of prime numbers less than a number x is roughly equal to x divided by the logarithm of x.

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

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

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

Science News
2004



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

Outline. What is HIGH PERFORMANCE MATHEMATICS?

1. Visual Data Mining in Mathematics.

- ✓ Fractals, Polynomials, Continued Fractions, Pseudospectra

2. High Precision Mathematics.

3. Integer Relation Methods.

- ✓ Chaos, Zeta and the Riemann Hypothesis, HexPi and Normality

4. Inverse Symbolic Computation.

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

---

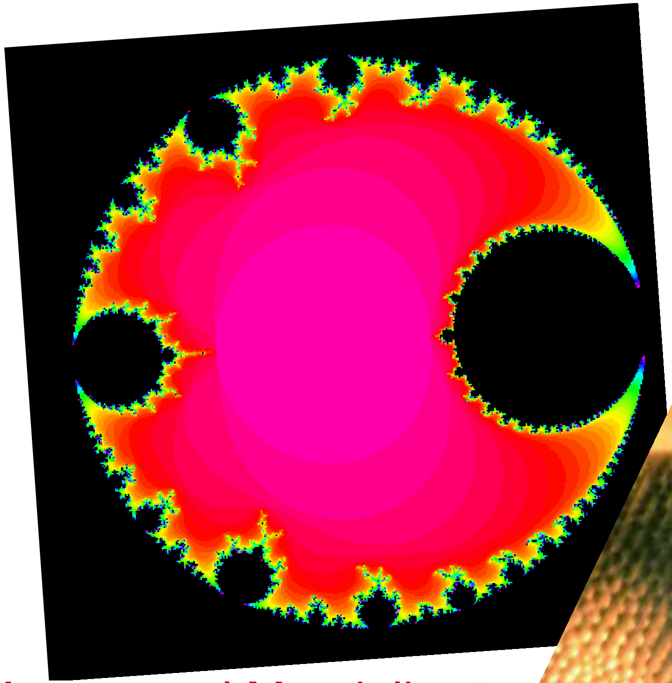
5. The Future is Here.

- ✓ **D-DRIVE**: Examples and Issues

6. Conclusion.

- ✓ Engines of Discovery. The 21st Century Revolution
  - ✓ Long Range Plan for HPC in Canada

Mathematical Data Mining



An unusual Mandelbrot parameterization

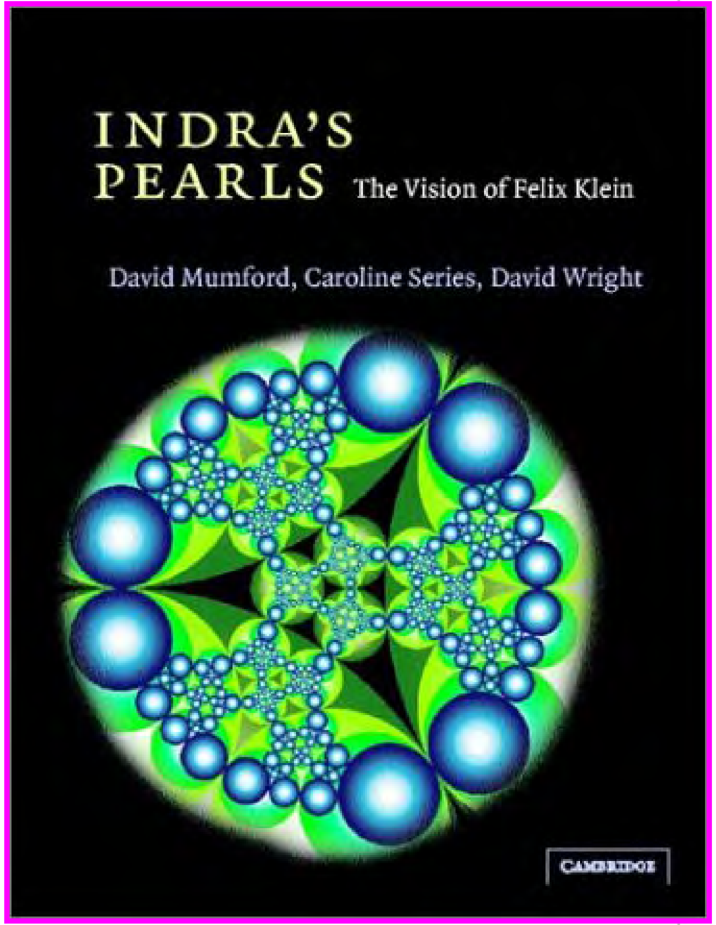
Various visual examples follow

- ✓ Roots of `1/-1' polynomials
- ✓ Ramanujan's fraction
- ✓ Sparsity and Pseudospectra

AK Peters, 2004
(CD in press)

Indra's Pearls

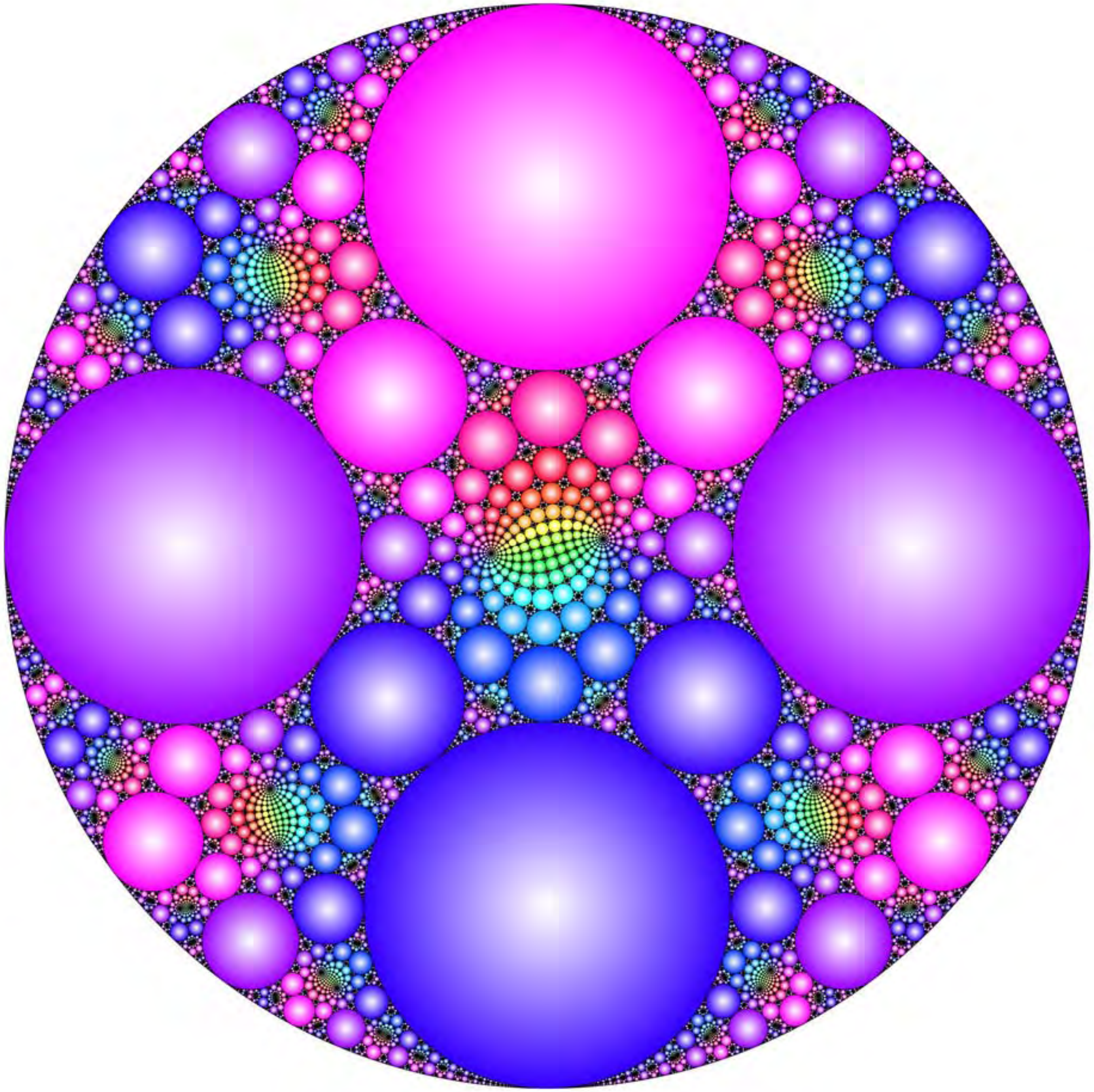
A merging of 19th and 21st Centuries



INDRA'S
PEARLS The Vision of Felix Klein

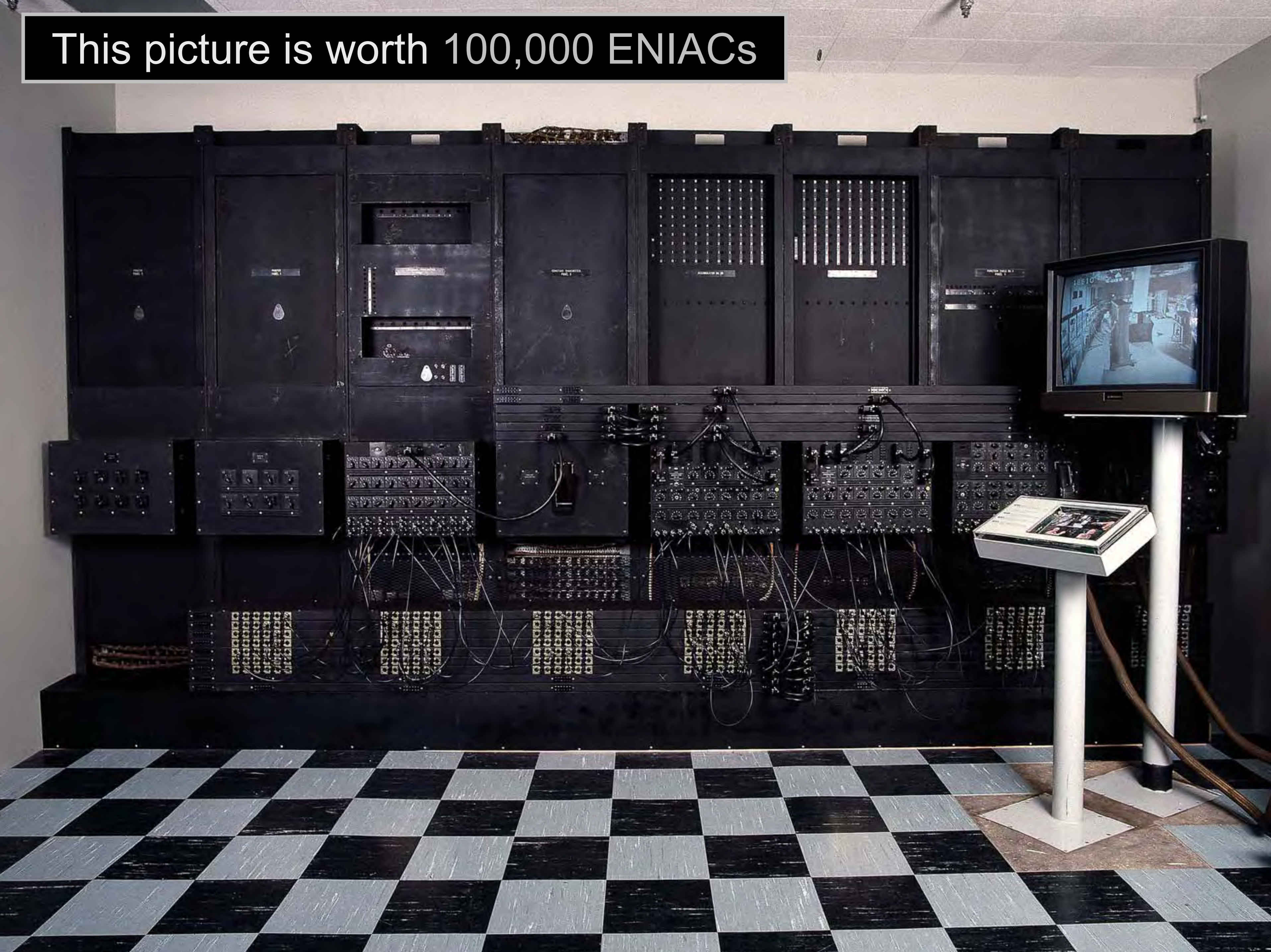
David Mumford, Caroline Series, David Wright

CAMBRIDGE



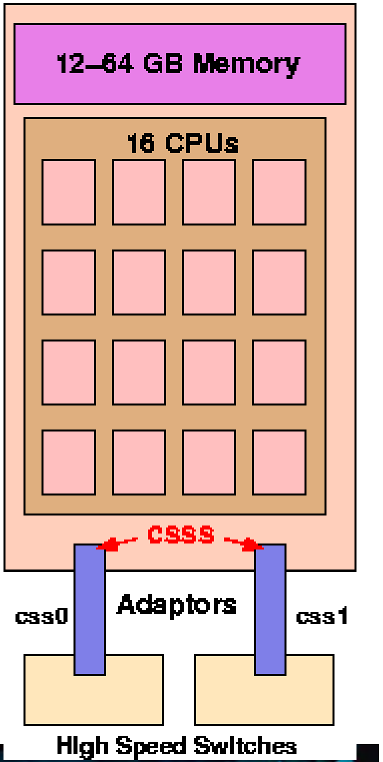
2002: http://klein.math.okstate.edu/IndrasPearls/

This picture is worth 100,000 ENIACs



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

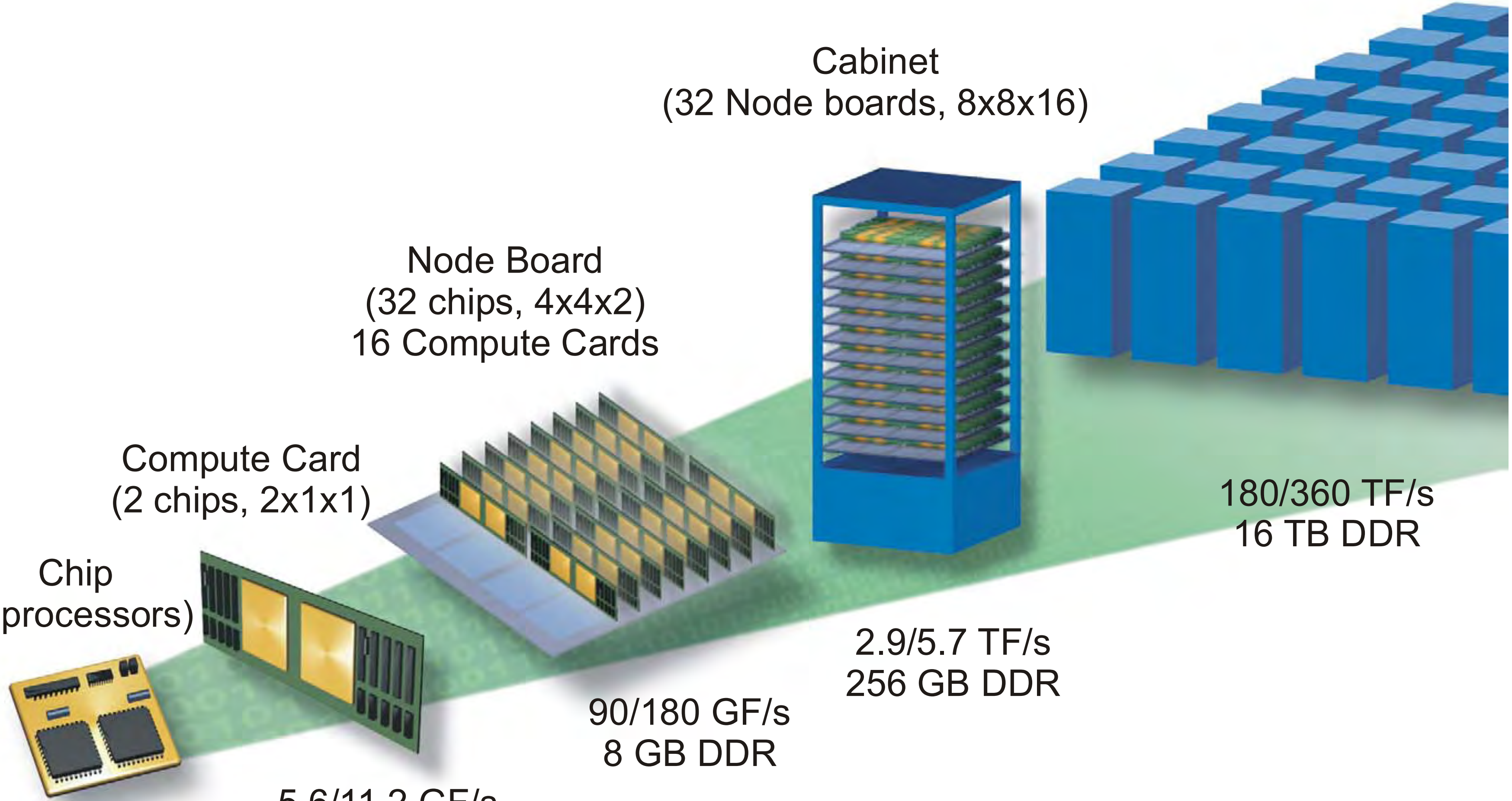
we need new software paradigms for `bigga-scale’ hardware



The present

Mathematical Immersive Reality
in Vancouver

IBM BlueGene/L system at LLNL



Chip
(2 processors)

2.8/5.6 GF/s
4 MB

Compute Card
(2 chips, 2x1x1)

5.6/11.2 GF/s
0.5 GB DDR

Node Board
(32 chips, 4x4x2)
16 Compute Cards

90/180 GF/s
8 GB DDR

Cabinet
(32 Node boards, 8x8x16)

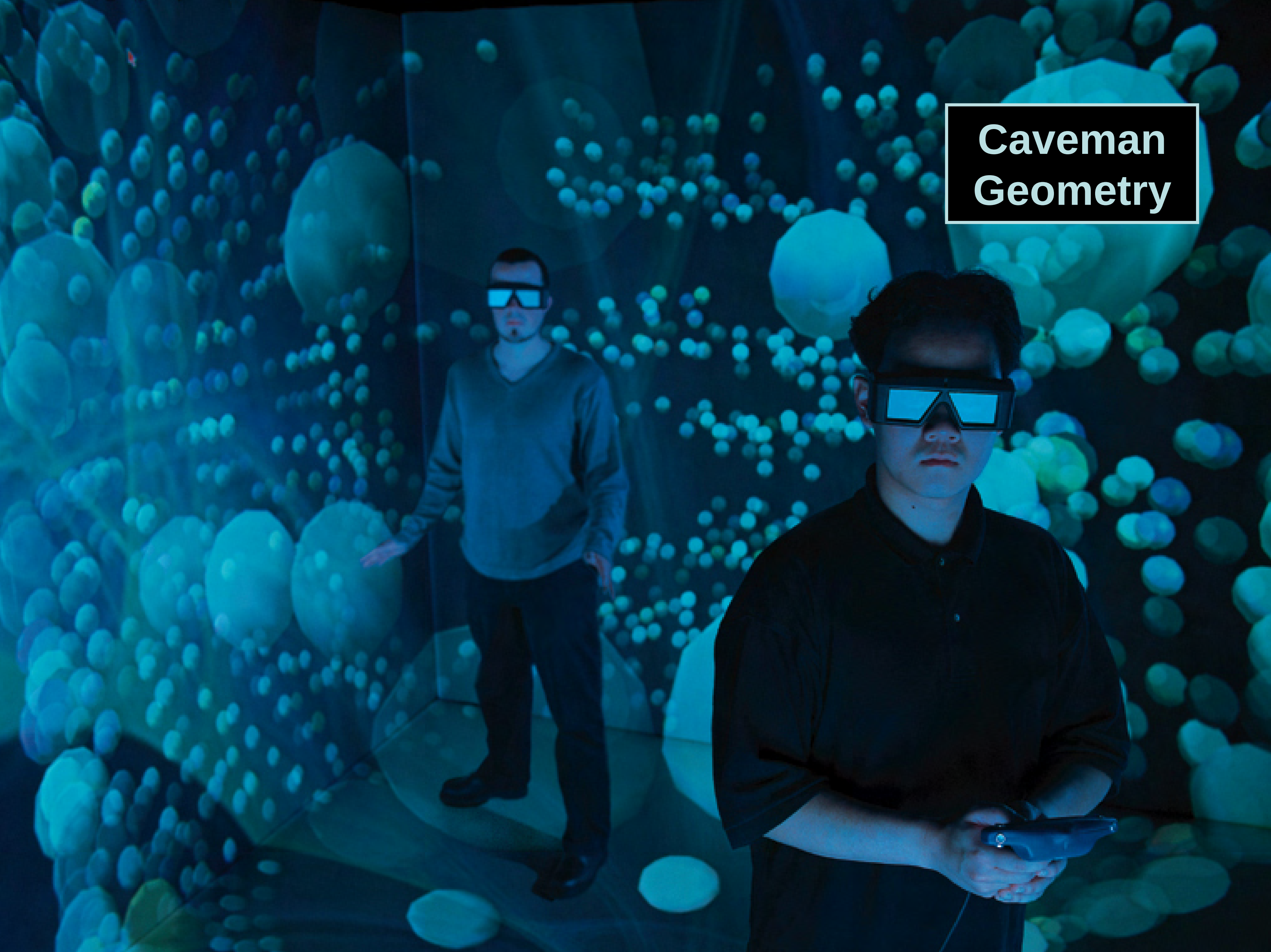
2.9/5.7 TF/s
256 GB DDR

System
(64 cabinets, 64x32x32)

180/360 TF/s
16 TB DDR

2^{17} cpu's

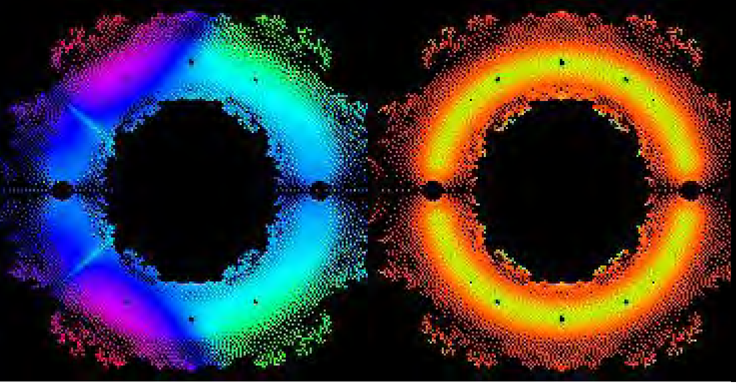
- has now run Linpack benchmark
- at over **120 Tflop/s**

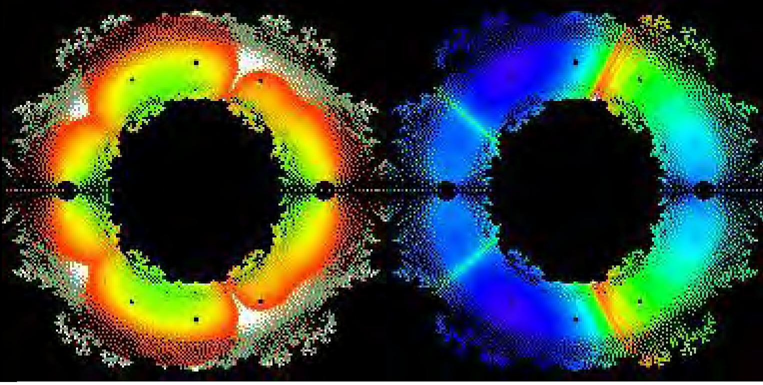


Caveman Geometry

Roots of Zeros

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





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

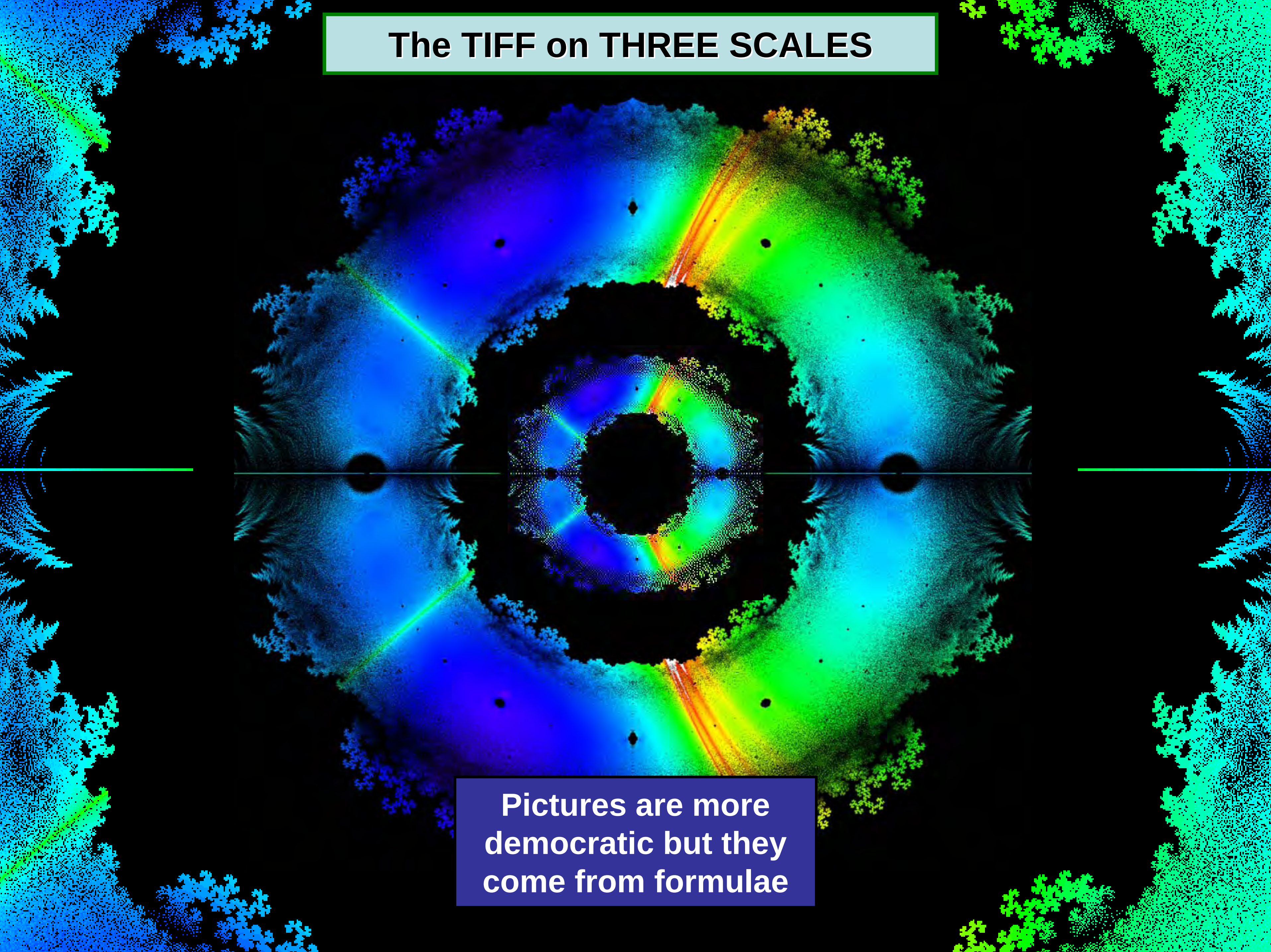
Coloration is by sensitivity of polynomials to slight variation around the values of the zeros. The color scale represents a normalized sensitivity to the range of values; red is insensitive to violet which is strongly sensitive.

- All zeros are pictured (at **3600 dpi**)
- Figure 1b is colored by their local density
- Figure 1d shows sensitivity relative to the **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

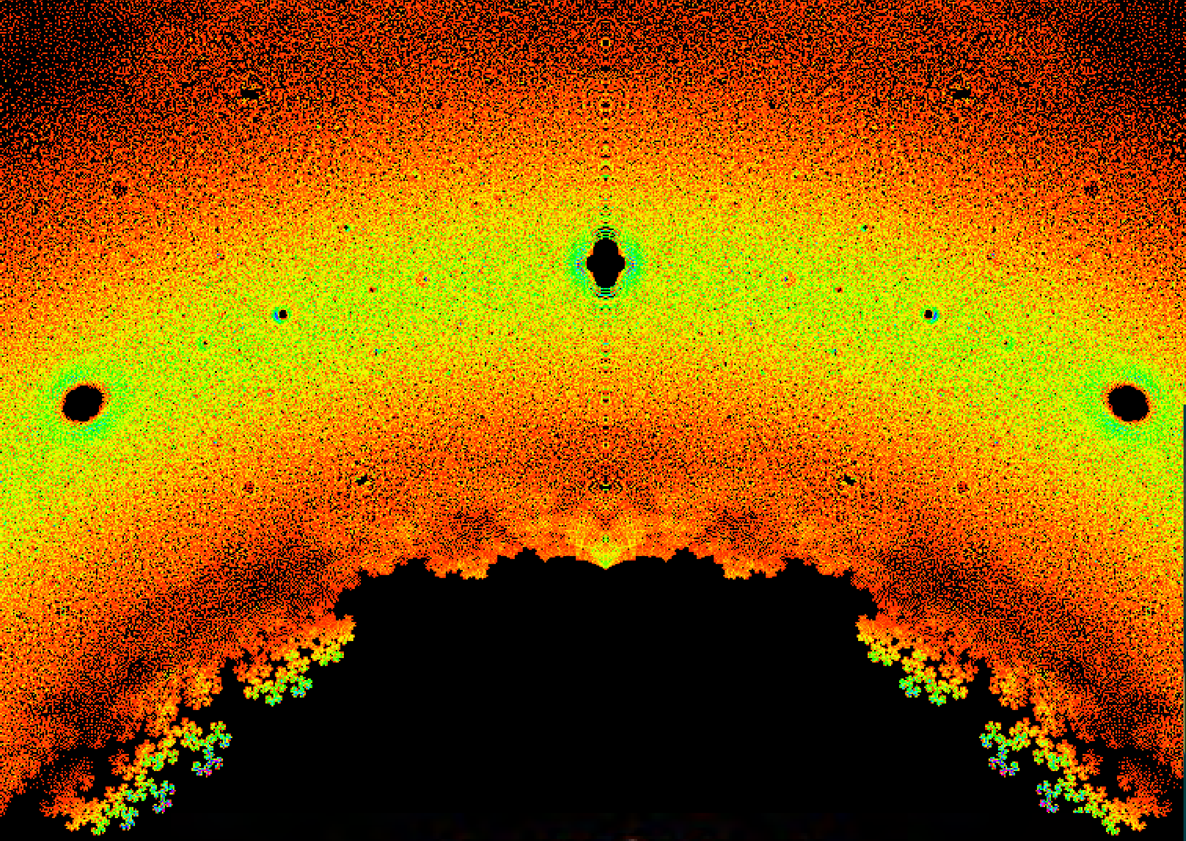
> *"The idea that we could make biology mathematical, I think, perhaps is not working, but what is happening, strangely enough, is that maybe mathematics will become biological!"* Greg Chaitin, Interview, 2000.

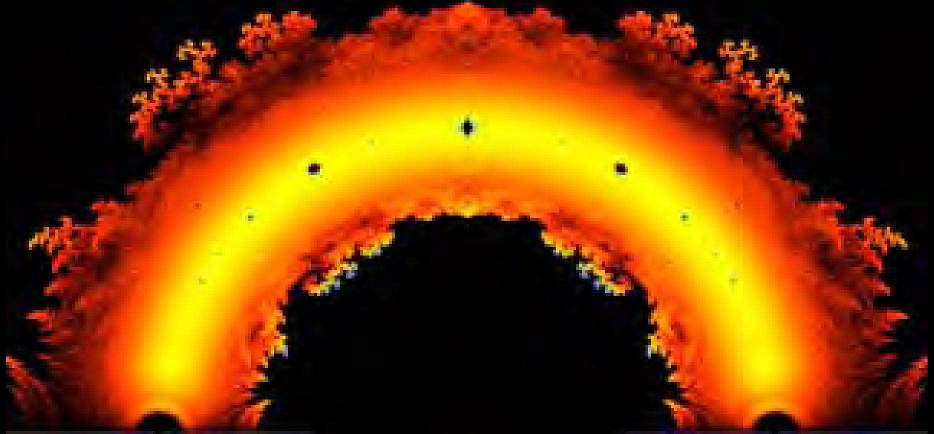
The TIFF on THREE SCALES

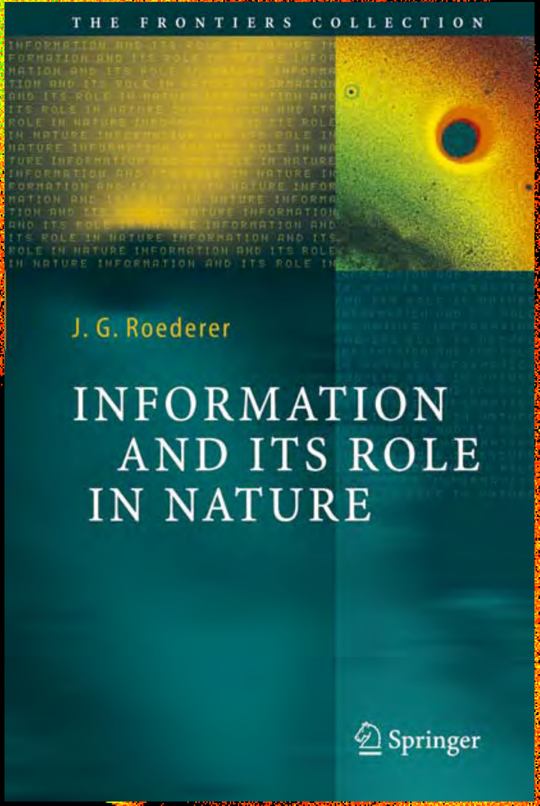


Pictures are more democratic but they come from formulae

and in the most stable colouring





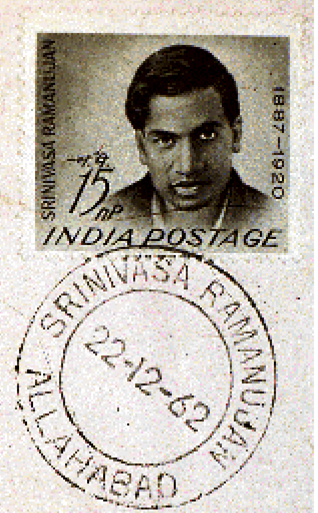


THE FRONTIERS COLLECTION

J. G. Roederer

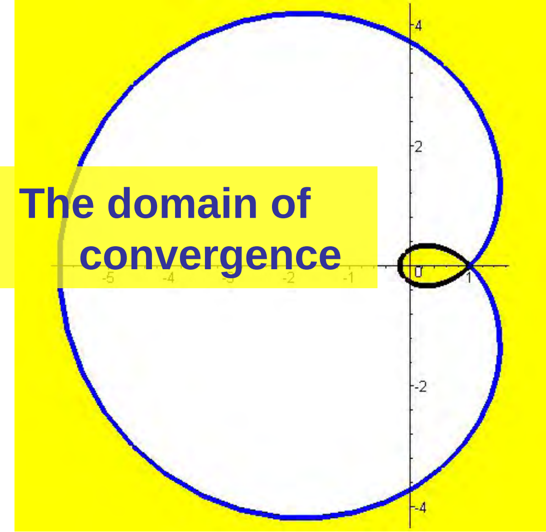
INFORMATION AND ITS ROLE IN NATURE

Springer



Ramanujan's Arithmetic-Geometric Continued fraction (CF)

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



The domain of convergence

A cardioid

- ☐ 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 just 4 places of $\mathcal{R}_1(1,1) = \log 2$

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

- ✓ The **scatterplot** revealed a precise **cardioid** where r=a/b.
  - ✓ which discovery it remained to prove?

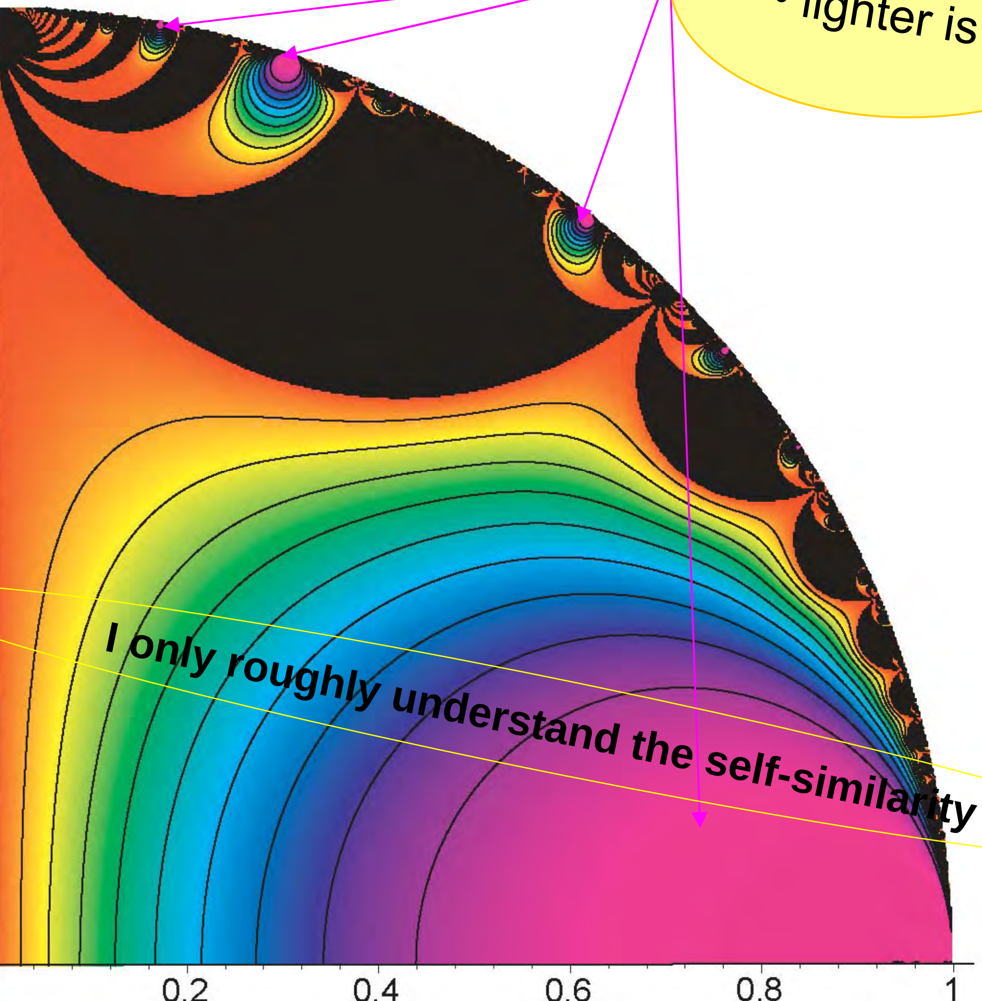
$r^2 - 2r\{2 - \cos(\theta)\} + 1 = 0$

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

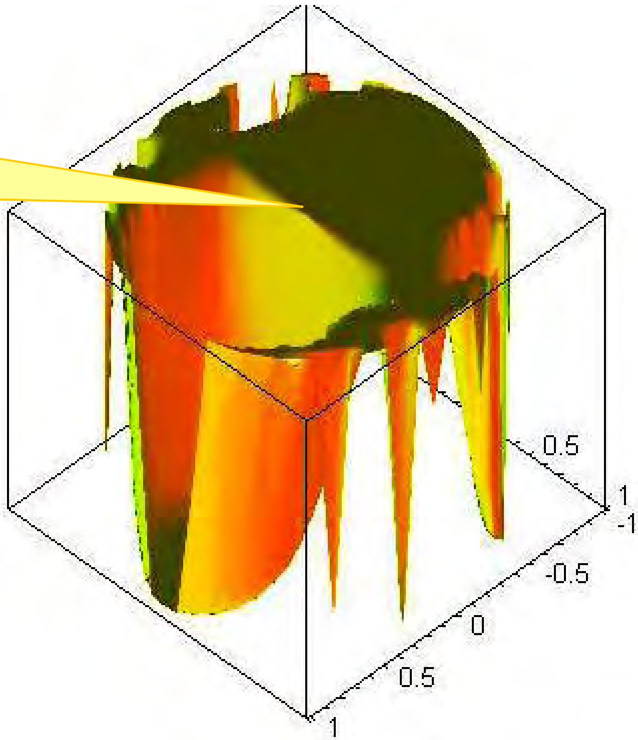
FRACTAL of a Modular Inequality

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

plots $\mathcal{R}$ in disk
- black exceeds 1
- lighter is lower



I only roughly understand the self-similarity

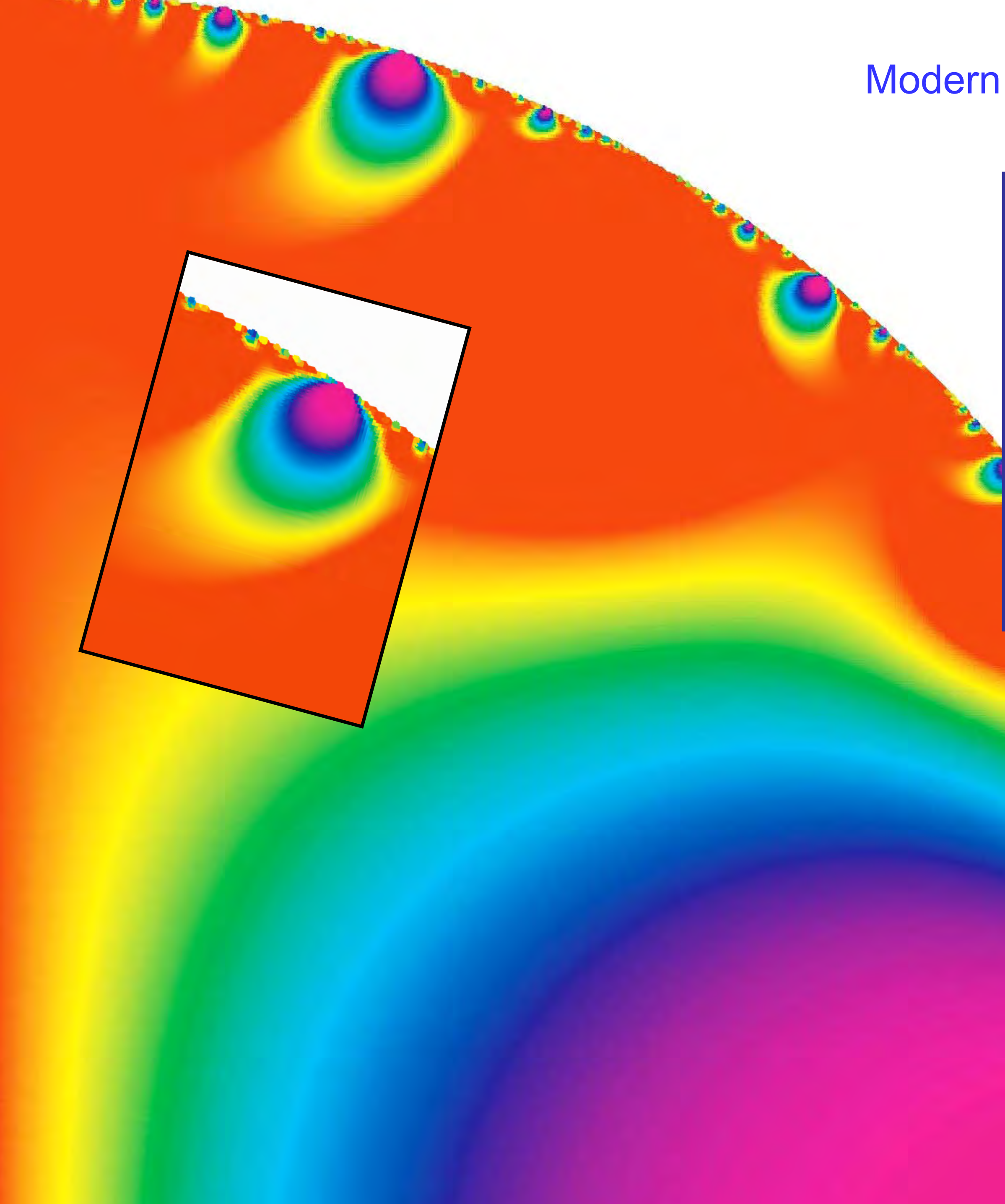


- ✓ related to Ramanujan's continued fraction
- ✓ took several hours to print
- ✓ Crandall/Apple has parallel print mode

Mathematics and the aesthetic

Modern approaches to an ancient affinity

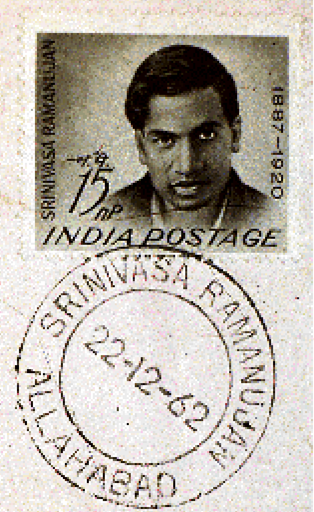
(CMS-Springer, 2005)



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

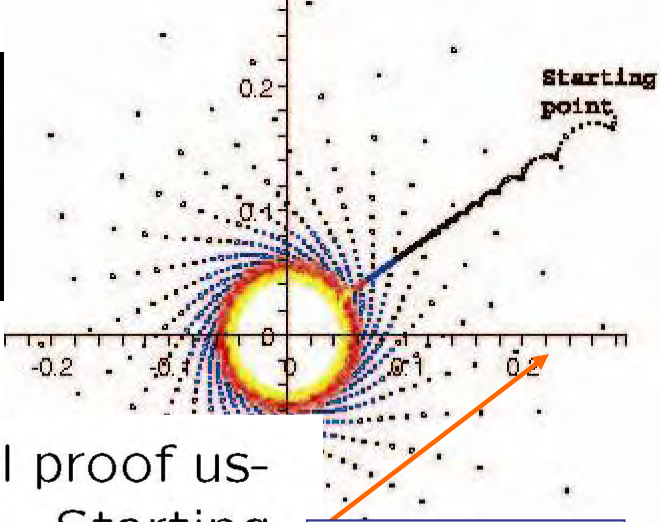
Oliver Heaviside (1850 - 1925)

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



Ramanujan's Arithmetic-Geometric Continued fraction

1. The Blackbox

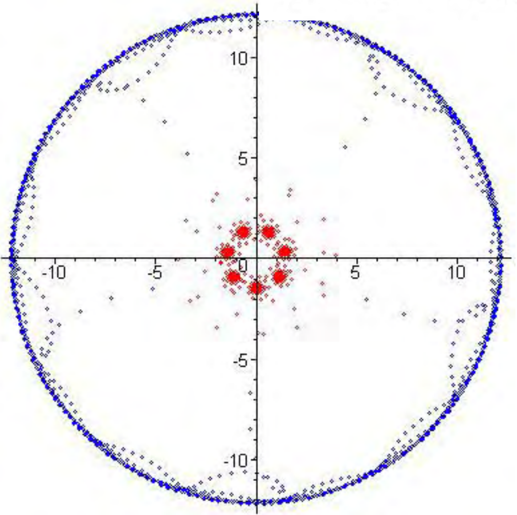


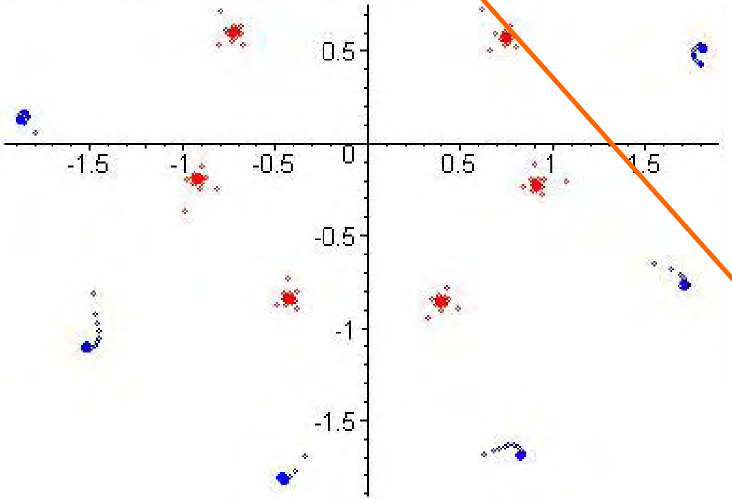
Six months later we had a beautiful proof using genuinely new dynamical results. Starting from the *dynamical system* $t_0 := t_1 := 1$:

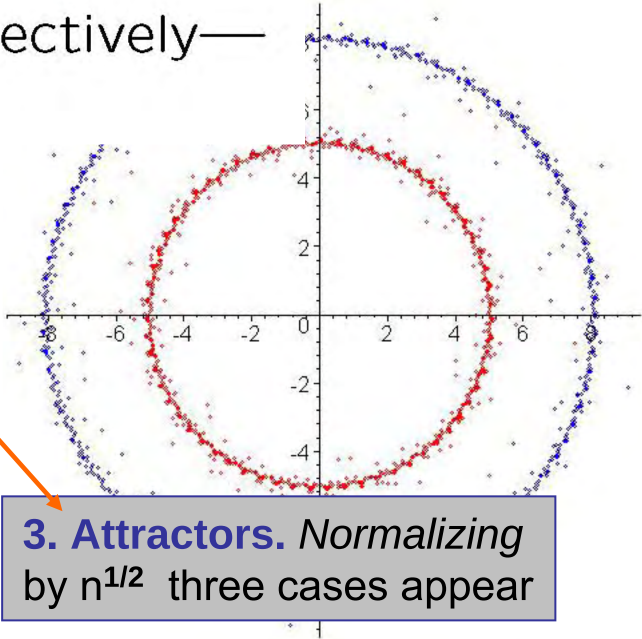
$$t_n \longleftarrow \frac{1}{n} t_{n-1} + \omega_{n-1}\left(1-\frac{1}{n}\right) t_{n-2},$$

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

2. Seeing convergence

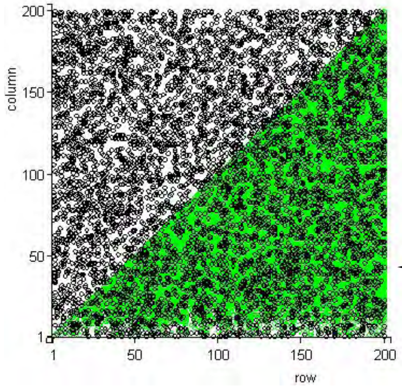




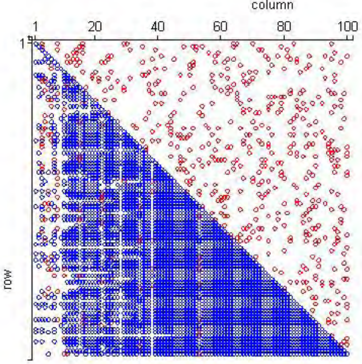


3. Attractors. *Normalizing* by $n^{1/2}$ three cases appear

Pseudospectra or Stabilizing Eigenvalues



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

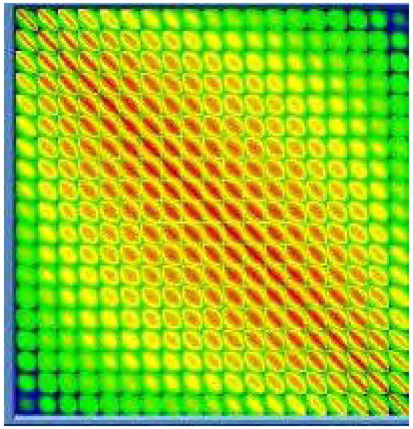


‘Large’ (10^5 to 10^8) Matrices must be seen

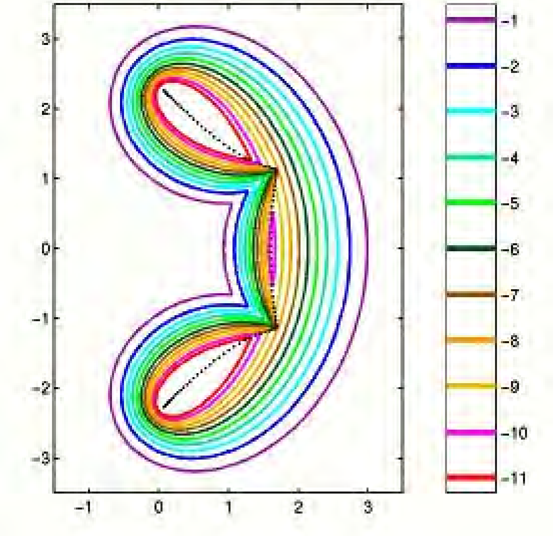
- ✓ sparsity and its preservation
- ✓ conditioning and ill-conditioning

- ✓ eigenvalues
- ✓ singular values (helping Google work)

A dense inverse



Pseudospectrum of a banded matrix



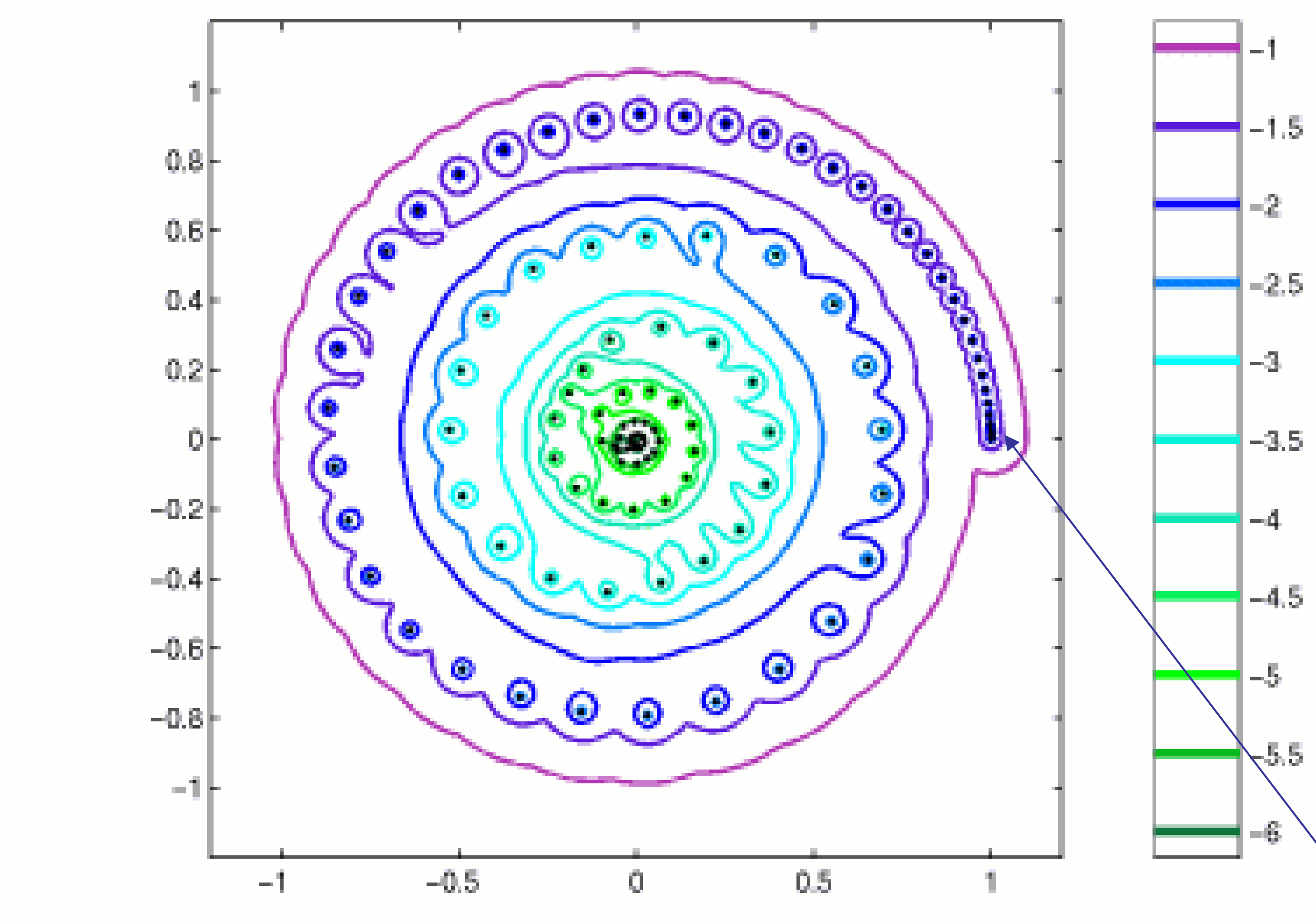
The ε-pseudospectrum of A
is: $$\sigma_\varepsilon(A) = \{x : \exists\lambda \,\text{s.t.}\, \|Ax - \lambda x\| \le \varepsilon\}$$

- ✓ for ε = 0 we recover the eigenvalues

- ✓ full pseudospectrum carries much more information

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

An Early Use of Pseudospectra (Landau, 1977)



$\varepsilon = 10^t$

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**

Generic Code Optimization

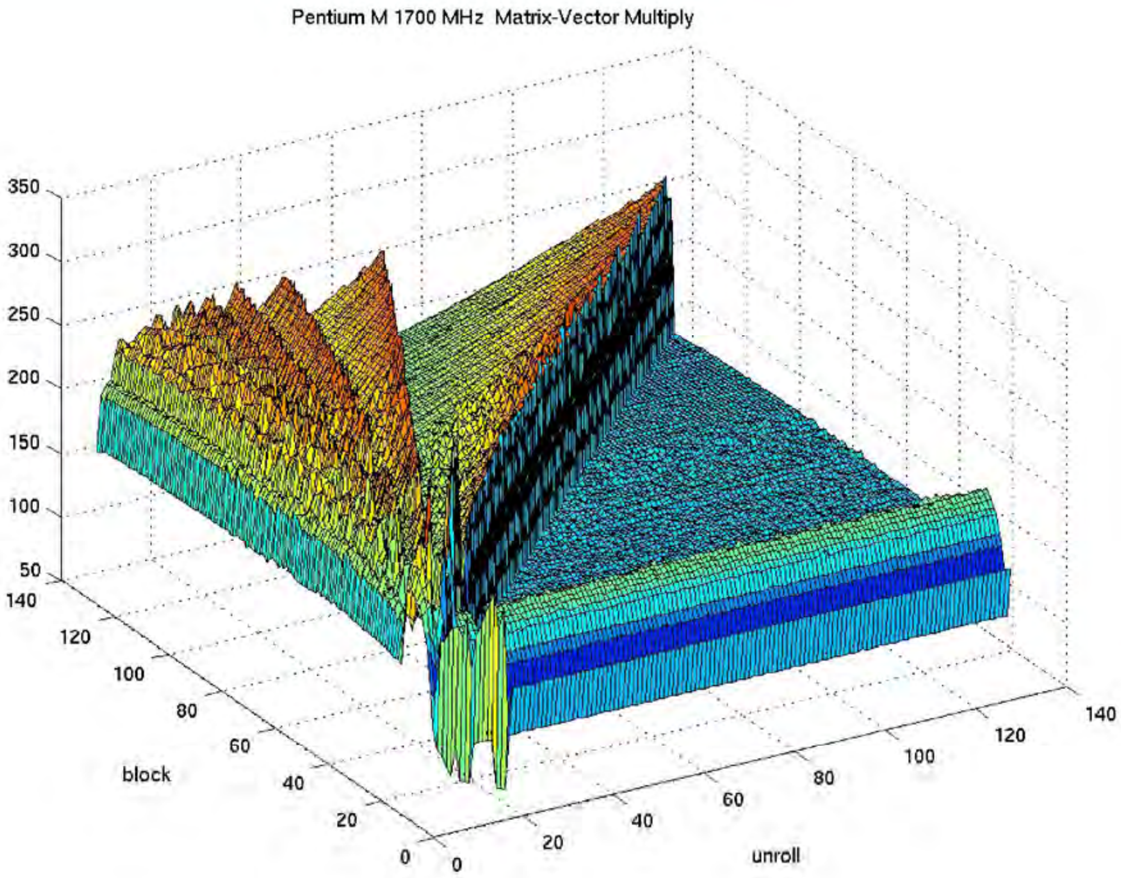
Experimentation with DGEMV (matrix-vector multiply):

128x128=16,384 cases.

Experiment took 30+ hours to run.

Best performance =
338 Mflop/s with
blocking=11
unrolling=11

Original performance =
232 Mflop/s



Visual Representation of Automatic Code Parallelization

Outline. What is HIGH PERFORMANCE MATHEMATICS?

1. **Visual Data Mining in Mathematics.**
    - ✓ **Fractals, Polynomials, Continued Fractions, Pseudospectra**
2. **High Precision Mathematics.**
3. **Integer Relation Methods.**
    - ✓ **Chaos, Zeta and the Riemann Hypothesis, HexPi and Normality**
4. **Inverse Symbolic Computation.**
    - ✓ **A problem of Knuth, $\pi/8$, Extreme Quadrature**
5. **The Future is Here.**
    - ✓ **Examples and Issues**
6. **Conclusion.**
    - ✓ **Engines of Discovery. The 21st Century Revolution**
        - ✓ **Long Range Plan for HPC in Canada**

A **WARMUP** Computer Proof

- ➢ Suppose we know that 1<α<10 and that α is an integer
  - **computing α to 1 significant place with a certificate** will prove the value of α. *Euclid's method* is basic to such ideas.
- ➢ Likewise, suppose we know α is *algebraic of degree d and length l*

(coefficient sum in absolute value)

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

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

Example (MAA, April 2005). Prove that

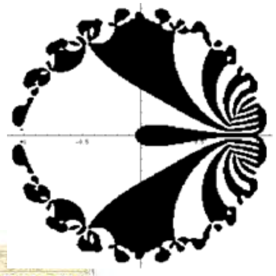
$$\int_{-\infty}^{\infty} \frac{y^2}{1+4\,y+y^6-2\,y^4-4\,y^3+2\,y^5+3\,y^2}\,dy = \pi$$

Proof. Purely **qualitative analysis** with partial fractions and arctans shows integral is π β where β is algebraic of degree *much* less than **100 (actually 6)**, length *much* less than **100,000,000**.

✓ With **P(x)=x-1** (D=1,L=2, d=6, **l=?**), this means *checking* the identity to **100** places is plenty **PROOF:** $|\beta - 1| < 1/(32l) \mapsto \beta = 1$

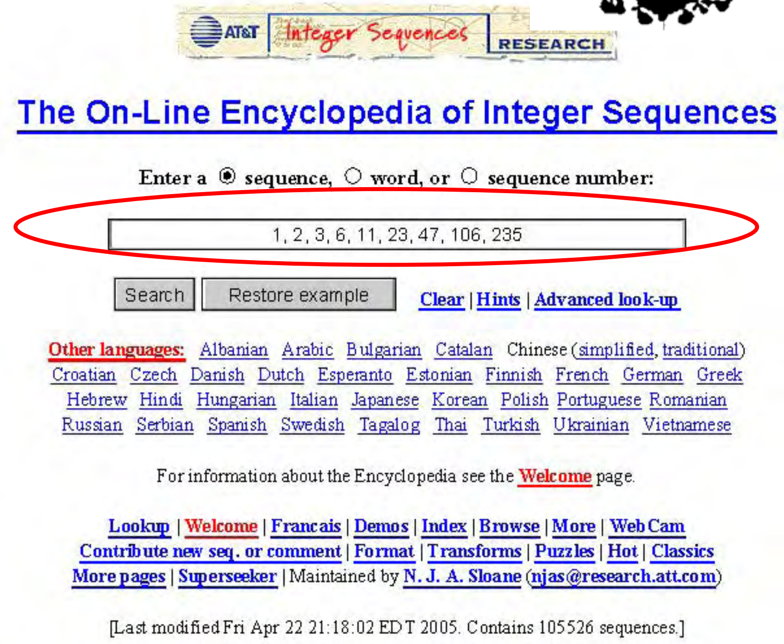
✓ A fully symbolic Maple proof followed. **QED**

Fast High Precision Numeric Computation (and Quadrature)



☐ 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



AT&T Integer Sequences RESEARCH

The On-Line Encyclopedia of Integer Sequences

Enter a ● sequence, ○ word, or ○ sequence number:

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

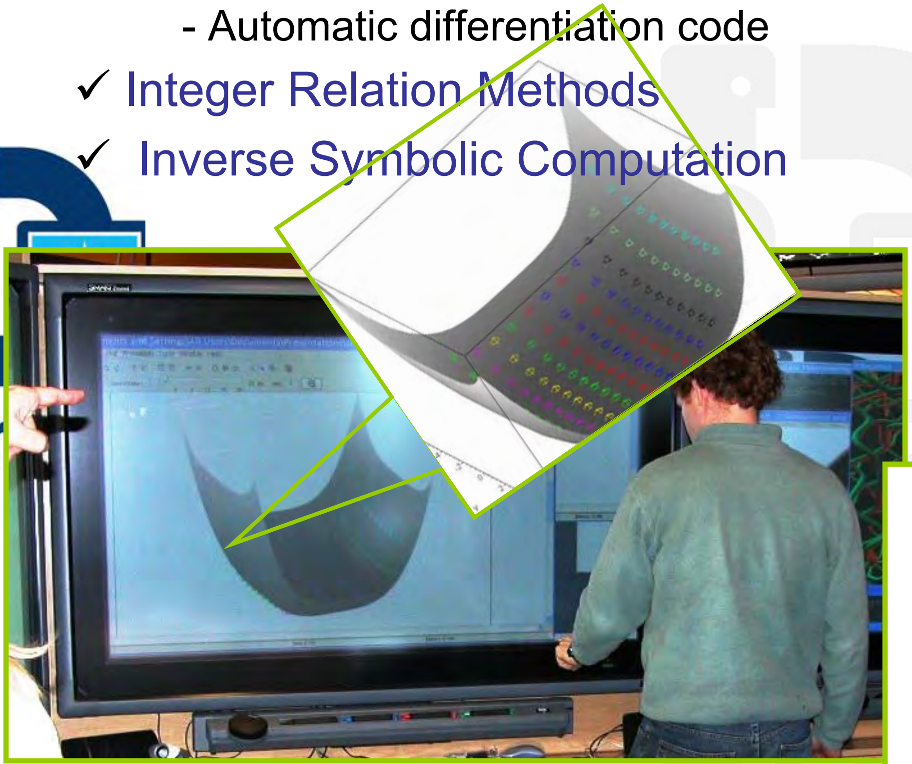
Search | Restore example | Clear | Hints | Advanced look-up

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

For information about the Encyclopedia see the Welcome page.

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

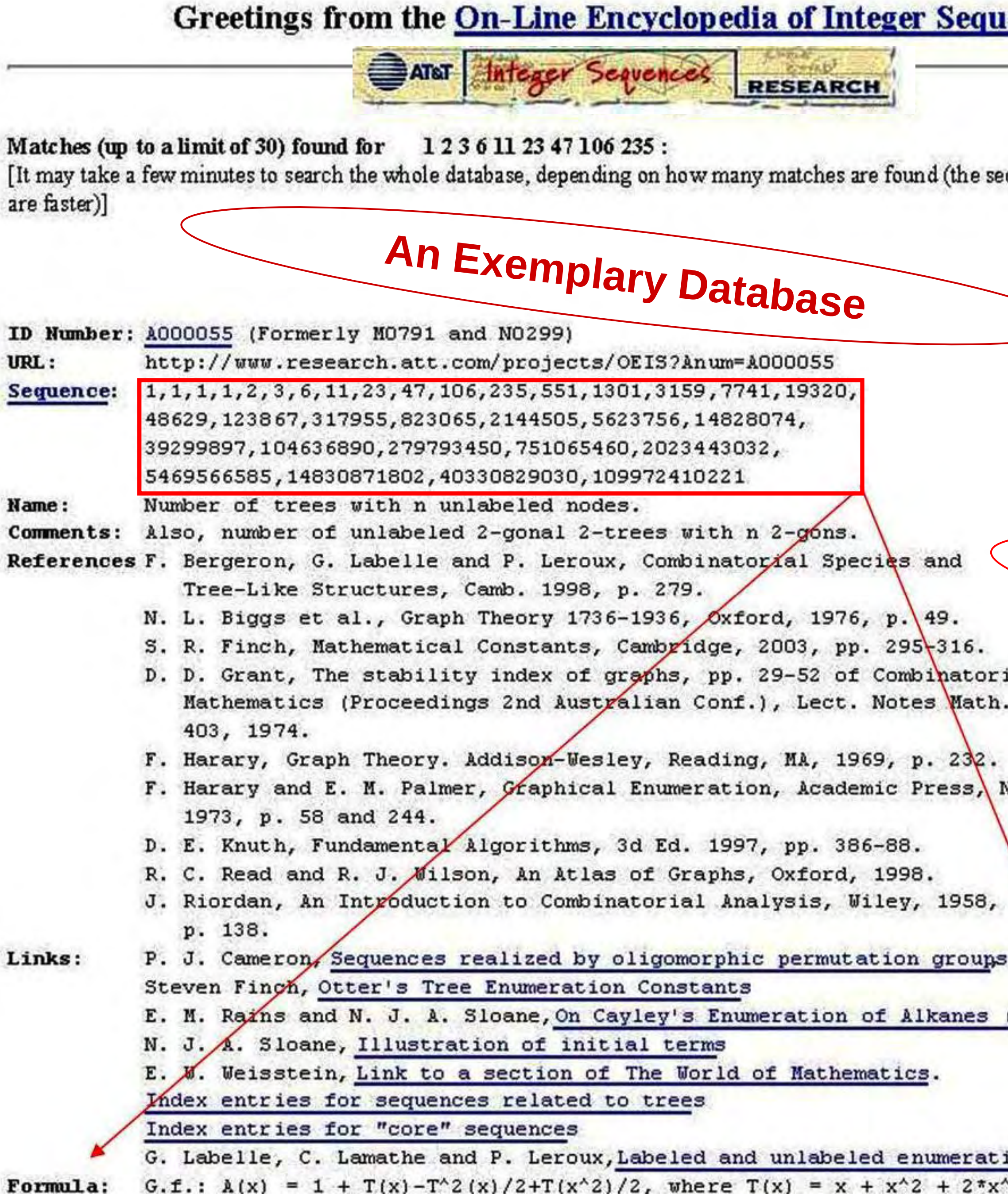
[Last modified Fri Apr 22 21:18:02 EDT 2005. Contains 105526 sequences.]



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

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 looku
are faster)]

```
ID Number: A000055 (Formerly M0791 and N0299)
URL:       http://www.research.att.com/projects/OEIS?Anum=A000055
Sequence:  1,1,1,1,2,3,6,11,23,47,106,235,551,1301,3159,7741,19320,
           48629,123867,317955,823065,2144505,5623756,14828074,
           39299897,104636890,279793450,751065460,2023443032,
           5469566585,14830871802,40330829030,109972410221
Name:      Number of trees with n unlabeled nodes.
Comments:  Also, number of unlabeled 2-gonal 2-trees with n 2-gons.
References F. Bergeron, G. Labelle and P. Leroux, Combinatorial Species and
             Tree-Like Structures, Camb. 1998, p. 279.
           N. L. Biggs et al., Graph Theory 1736-1936, Oxford, 1976, p. 49.
           S. R. Finch, Mathematical Constants, Cambridge, 2003, pp. 295-316.
           D. D. Grant, The stability index of graphs, pp. 29-52 of Combinatorial
             Mathematics (Proceedings 2nd Australian Conf.), Lect. Notes Math.
             403, 1974.
           F. Harary, Graph Theory. Addison-Wesley, Reading, MA, 1969, p. 232.
           F. Harary and E. M. Palmer, Graphical Enumeration, Academic Press, NY,
             1973, p. 58 and 244.
           D. E. Knuth, Fundamental Algorithms, 3d Ed. 1997, pp. 386-88.
           R. C. Read and R. J. Wilson, An Atlas of Graphs, Oxford, 1998.
           J. Riordan, An Introduction to Combinatorial Analysis, Wiley, 1958,
             p. 138.
Links:     P. J. Cameron, Sequences realized by oligomorphic permutation groups J. Integ. Seqs. 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-tree
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 + ...
```

An Exemplary Database

Integrated real time use

- moderated
- 100,000 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'

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

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

Outline. What is HIGH PERFORMANCE MATHEMATICS?

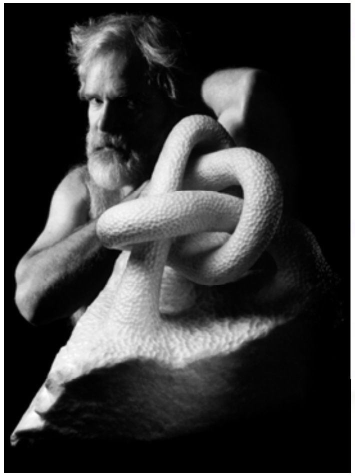
1. Visual Data Mining in Mathematics.
   - ✓ Fractals, Polynomials, Continued Fractions, Pseudospectra
2. High Precision Mathematics.
3. Integer Relation Methods.
   - ✓ Chaos, Zeta & Riemann Hypothesis, HexPi &Normality
4. Inverse Symbolic Computation.
   - ✓ A problem of Knuth, $\pi/8$, Extreme Quadrature
5. The Future is Here.
   - ✓ Examples and Issues
6. Conclusion.
   - ✓ Engines of Discovery. The 21st Century Revolution
     - ✓ Long Range Plan for HPC in Canada

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

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

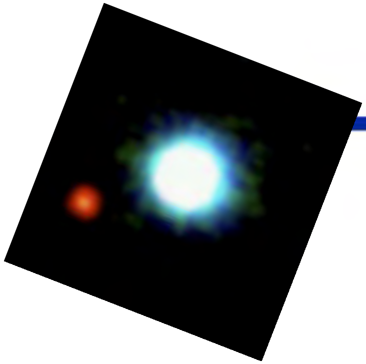


- At the present time, the PSLQ algorithm of mathematician-sculptor Helaman Ferguson is the best-known integer relation algorithm.
- PSLQ was named one of ten “algorithms of the century” by *Computing in Science and Engineering*.
- High precision arithmetic software is required: at least d x n digits,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

An Immediate Use

To see if α is algebraic of degree N, consider $(1,\alpha,\alpha^2,\ldots,\alpha^N)$

Application of PSLQ: Bifurcation Points in Chaos Theory



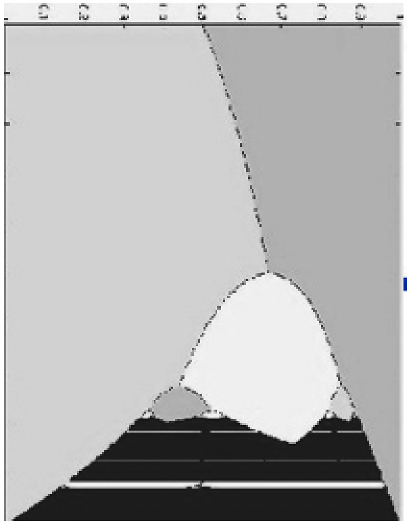
B_3 = 3.54409035955… is third bifurcation point of the logistic iteration of chaos theory:

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

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.

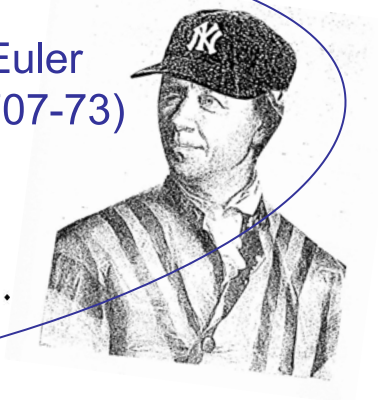
- The proofs use **Groebner basis** techniques
- Another useful part of the HPM toolkit

PSLQ and Zeta

Riemann
(1826-66)

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

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



Euler
(1707-73)

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

1

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

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

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

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

2

2. reduced as hoped

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

3

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

3. was easily **computer proven** (Wilf-Zeilberger)

If this were a philosophy talk I should discuss the following two quotes and defend our philosophy of mathematics:

Abstract of the future *We show in a certain precise sense that the* ***Goldbach Conjecture*** *is true with probability larger than 0.99999 and that its complete truth could be determined with a budget of 10 billion.*

"Secure Mathematical Knowledge"

"It is a waste of money to get absolute certainty, unless the conjectured identity in question is known to imply the Riemann Hypothesis."

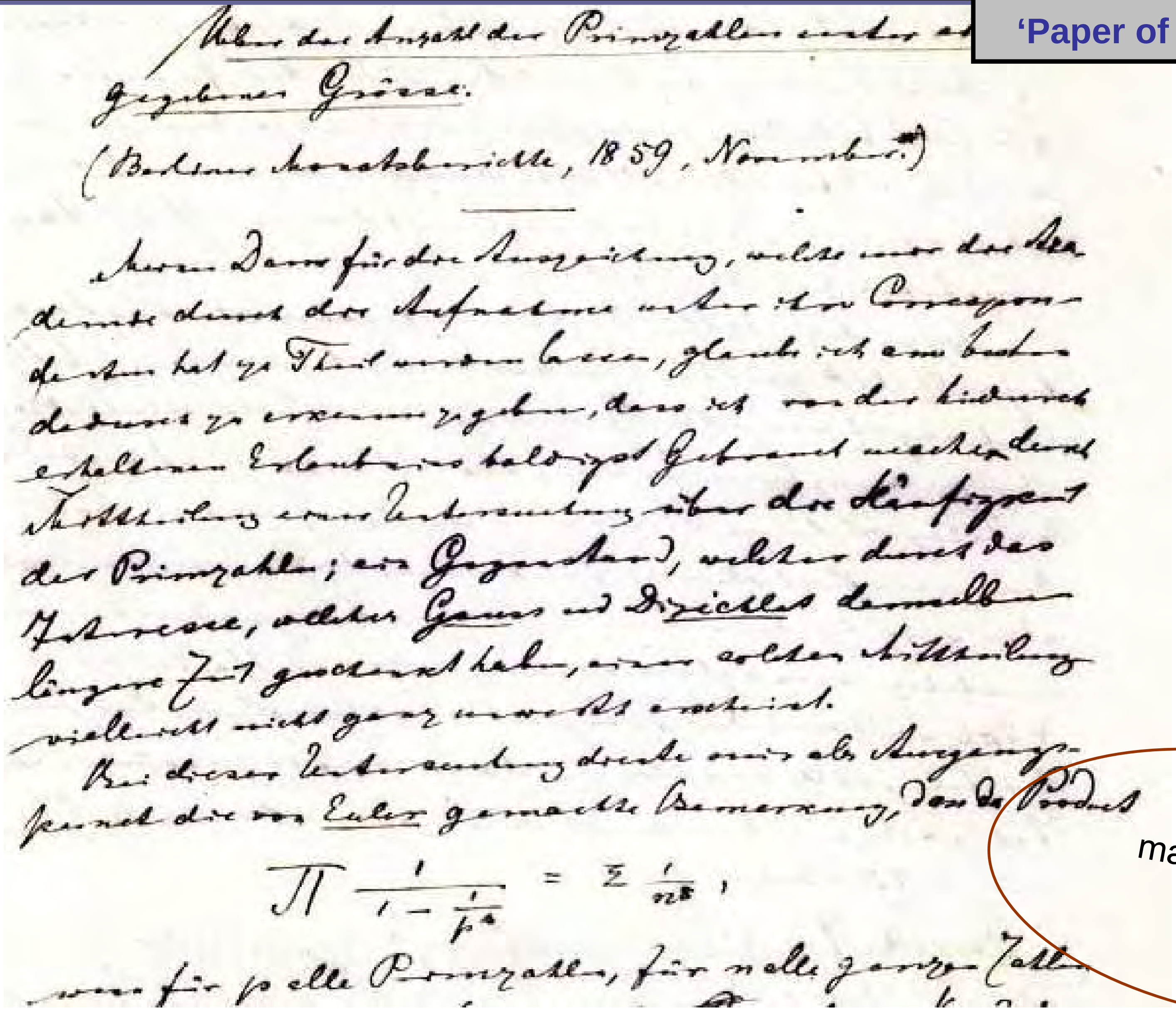
Doron Zeilberger, 1993

- ✓ **Goldbach**: every even number (>2) is a sum of two primes?
- ✓ So we will look at the **Riemann Hypothesis** …

Uber die Anzahl der Primzahlen unter einer Gegebenen Grosse

On the number of primes less than a given quantity

Riemann’s six page 1859
‘Paper of the Millennium’?



Ueber die Anzahl der Primzahlen unter ei

gegebenen Grösse.

(Berliner Monatsberichte, 1859, November.*)

Meinen Dank für die Auszeichnung, welche mir die Akademie durch die Aufnahme unter ihre Correspondenten hat zu Theil werden lassen, glaube ich am besten dadurch zu erkennen zu geben, dass ich von der hierdurch erhaltenen Erlaubniss baldigst Gebrauch mache durch Mittheilung einer Untersuchung über die Häufigkeit der Primzahlen; ein Gegenstand, welcher durch das Interesse, welches Gauss und Dirichlet demselben längere Zeit geschenkt haben, einer solchen Mittheilung vielleicht nicht ganz unwerth erscheint.

Bei dieser Untersuchung diente mir als Ausgangspunkt die von Euler gemachte Bemerkung, dass das Product

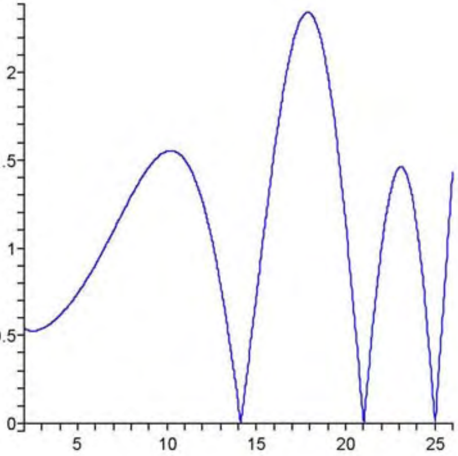
$$\prod \frac{1}{1-\frac{1}{p^s}} = \sum \frac{1}{n^s},$$

wenn für p alle Primzahlen, für n alle ganzen Zahl

RH is so important because it yields precise results on distribution and behaviour of primes

Euler’s product makes the key link between **primes and ζ**

The Modulus of Zeta and the **Riemann Hypothesis** (A Millennium Problem)



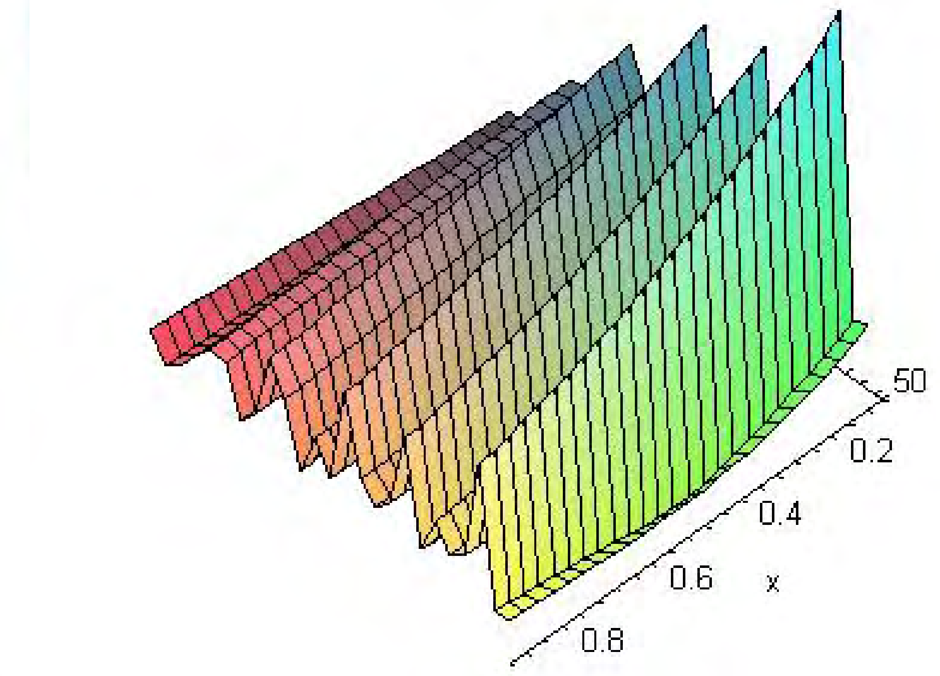
The imaginary parts of first 4 zeroes are:

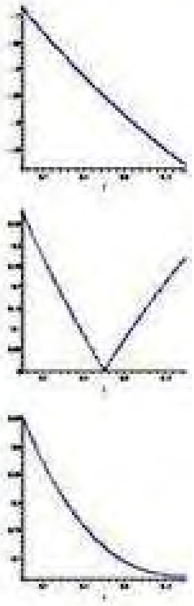
14.134725142
21.022039639

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)





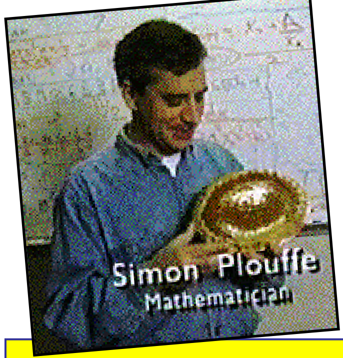
Curves at
and around
the 1st zero
. . . .

'All non-real zeros have real part one-half'

(The Riemann Hypothesis)

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

PSLQ and Hex Digits of Pi



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

My brother made the observation that this log formula allows one to compute binary digits of log 2 *without* knowing the previous ones! (a **BBP formula**)

Bailey, Plouffe and he hunted for such a formula for Pi. Three months later **the computer** - doing **bootstrapped PSLQ** hunts - **returned**:

$$\pi = 4F(1/4, 5/4; 1; -1/4) + 2\arctan(1/2) - \log 5$$

- this reduced to

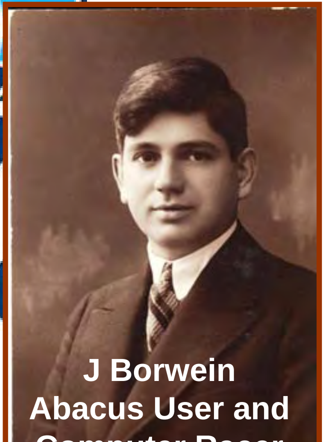
$$\pi = \sum_{i=0}^{\infty} \frac{1}{16^i} \left(\frac{4}{8i+1} - \frac{2}{8i+4} - \frac{1}{8i+5} - \frac{1}{8i+6} \right)$$

which *Maple*, *Mathematica* and humans can easily prove.

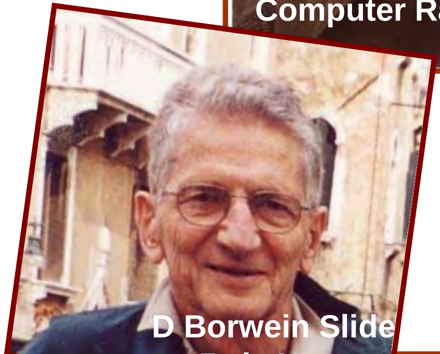
✓ A triumph for "**reverse engineered mathematics"** - algorithm design

✓ No such formula exists base-ten (provably)

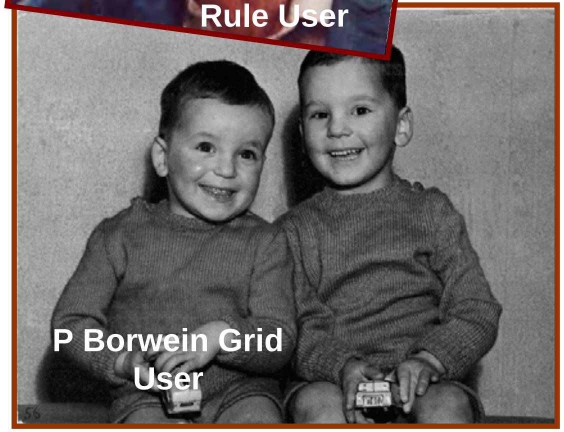
The pre-designed Algorithm ran the next day



J Borwein Abacus User and Computer Racer



D Borwein Slide Rule User



P Borwein Grid User

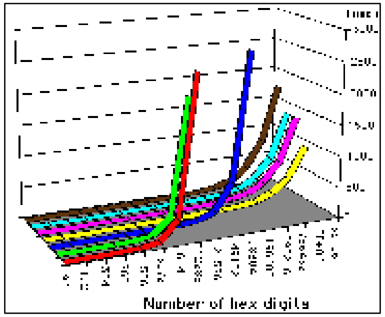
ALGORITHMIC PROPERTIES

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

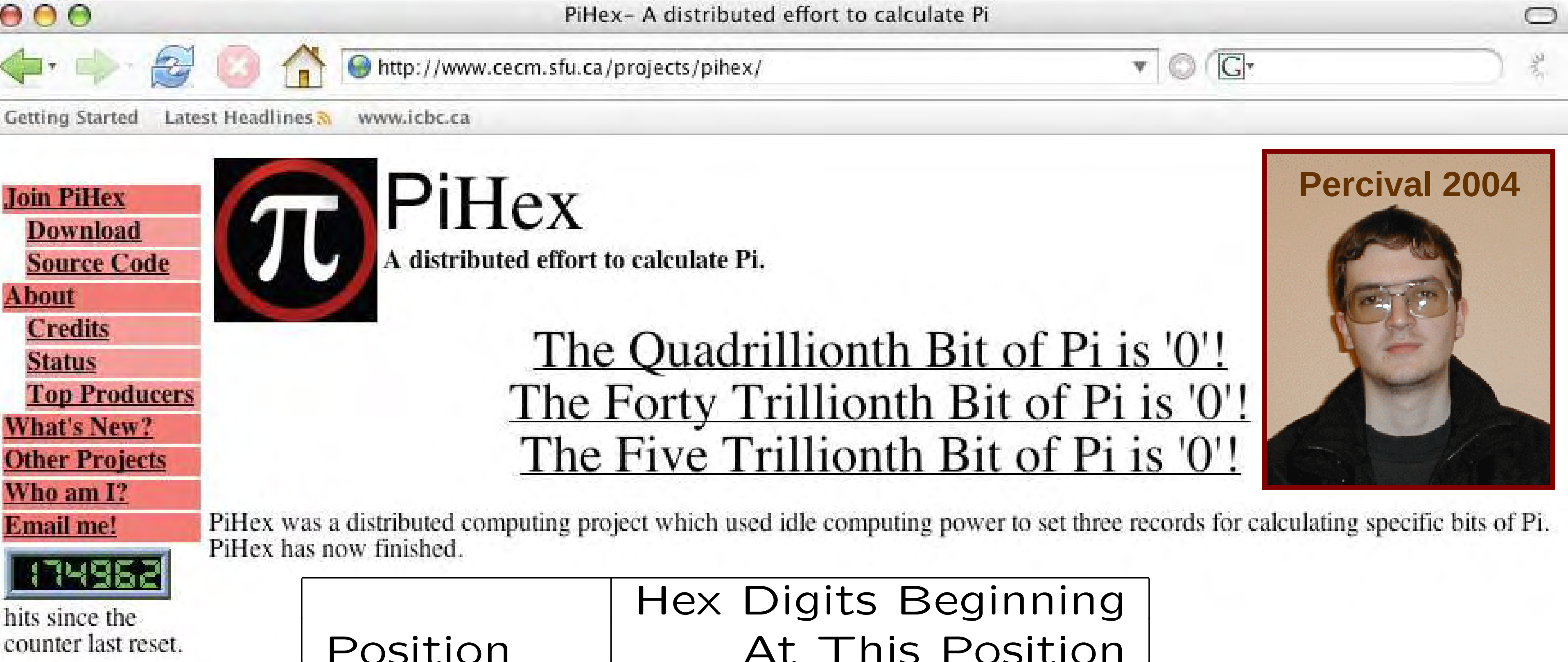
(2) is implementable on any modern computer;

(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.



PiHex- A distributed effort to calculate Pi

http://www.cecm.sfu.ca/projects/pihex/

Getting Started Latest Headlines www.icbc.ca

- Join PiHex
  - Download
  - Source Code
- About
  - Credits
  - Status
  - Top Producers
- What's New?
- Other Projects
- Who am I?
- Email me!

174962 hits since the counter last reset.

PiHex

A distributed effort to calculate Pi.

Percival 2004

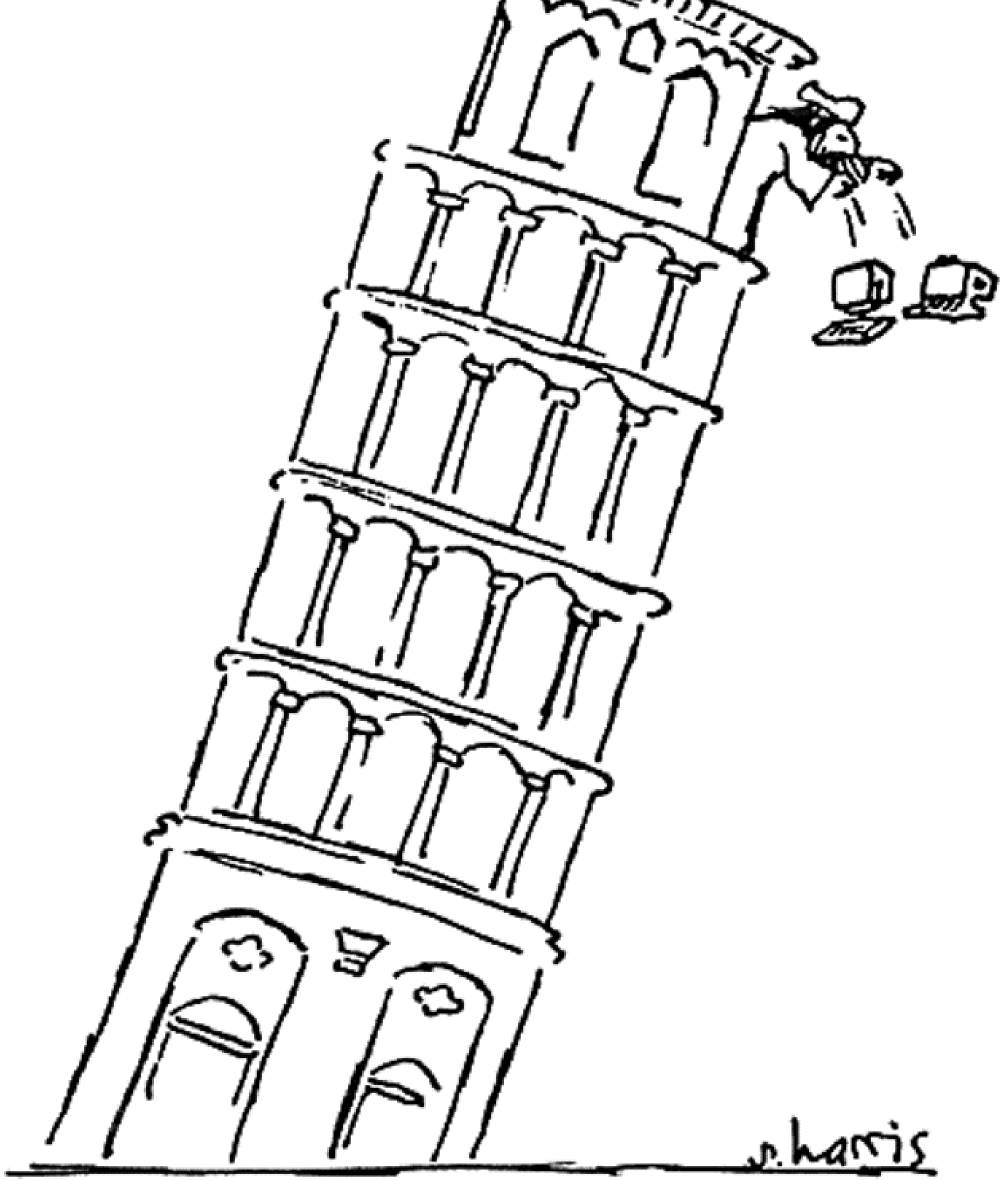
The Quadrillionth Bit of Pi is '0'!
The Forty Trillionth Bit of Pi is '0'!
The Five Trillionth Bit of Pi is '0'!

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.

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
1.25×10^{12}	07E45733CC790B
2.5×10^{14}	E6216B069CB6C1

Undergraduate
Colin Percival's
Grid
Computation
(PiHex) rivaled
Finding Nemo

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



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

2. High Precision Mathematics.

3. Integer Relation Methods.

✓ Chaos, Zeta and the Riemann Hypothesis, HexPi and Normality

4. Inverse Symbolic Computation.

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

5. The Future is Here.

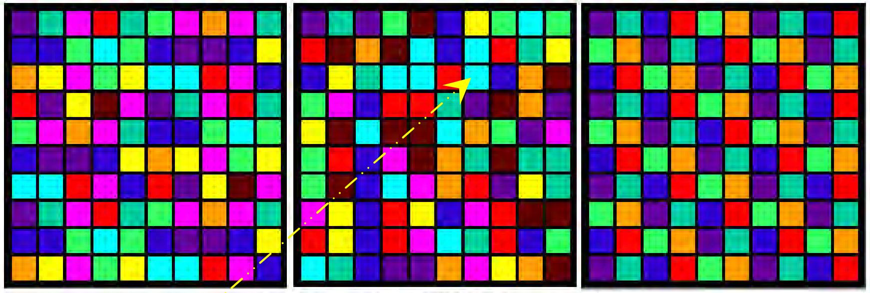
✓ Examples and Issues

6. Conclusion.

✓ Engines of Discovery. The 21st Century Revolution

  ✓ Long Range Plan for HPC in Canada

An Inverse and a Color Calculator

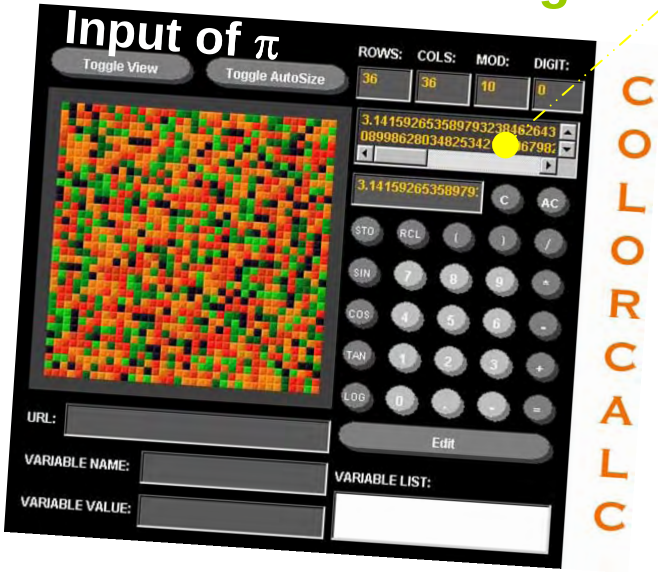


Archimedes: 223/71 < π < 22/7

Inverse Symbolic Computation

- “**Inferring symbolic 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 **identify** in Maple and **Recognize** in Mathematica



Input of π

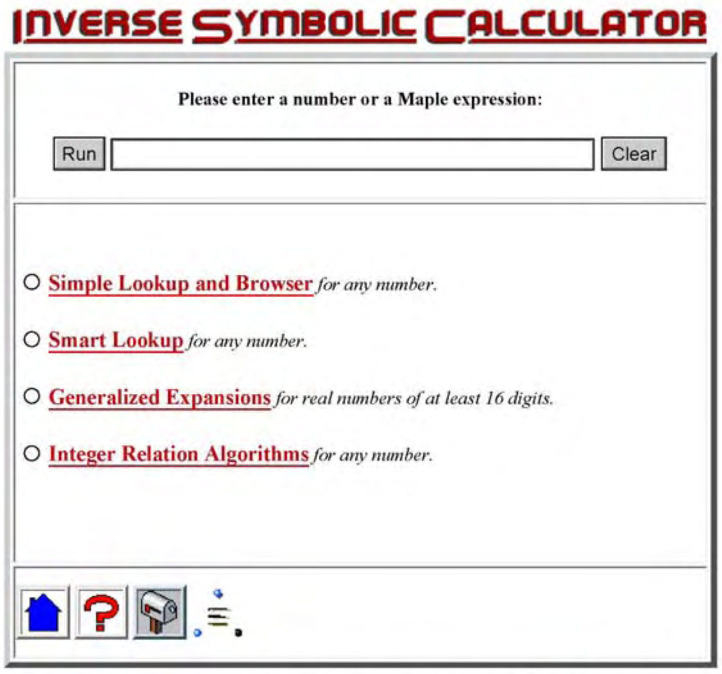
ROWS: 36
COLS: 36
MOD: 10
DIGIT: 0

3.14159265358979323846264308998628034825342
67982

3.14159265358979:

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

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



INVERSE SYMBOLIC CALCULATOR

Please enter a number or a Maple expression:

○ 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.*

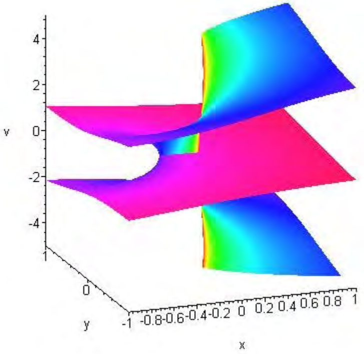
Expressions that are **not** numeric like ln(Pi*sqrt(2)) are evaluated in Maple in symbolic form first, followed by a floating point evaluation followed by a lookup.

Knuth’s Problem – we can know the answer first

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

The answer is **Lambert’s W** which solves

W exp(W) = x



W’s **Riemann** surface

Donald Knuth* asked for a closed form evaluation of:

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

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

† ISC is shown on next slide

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

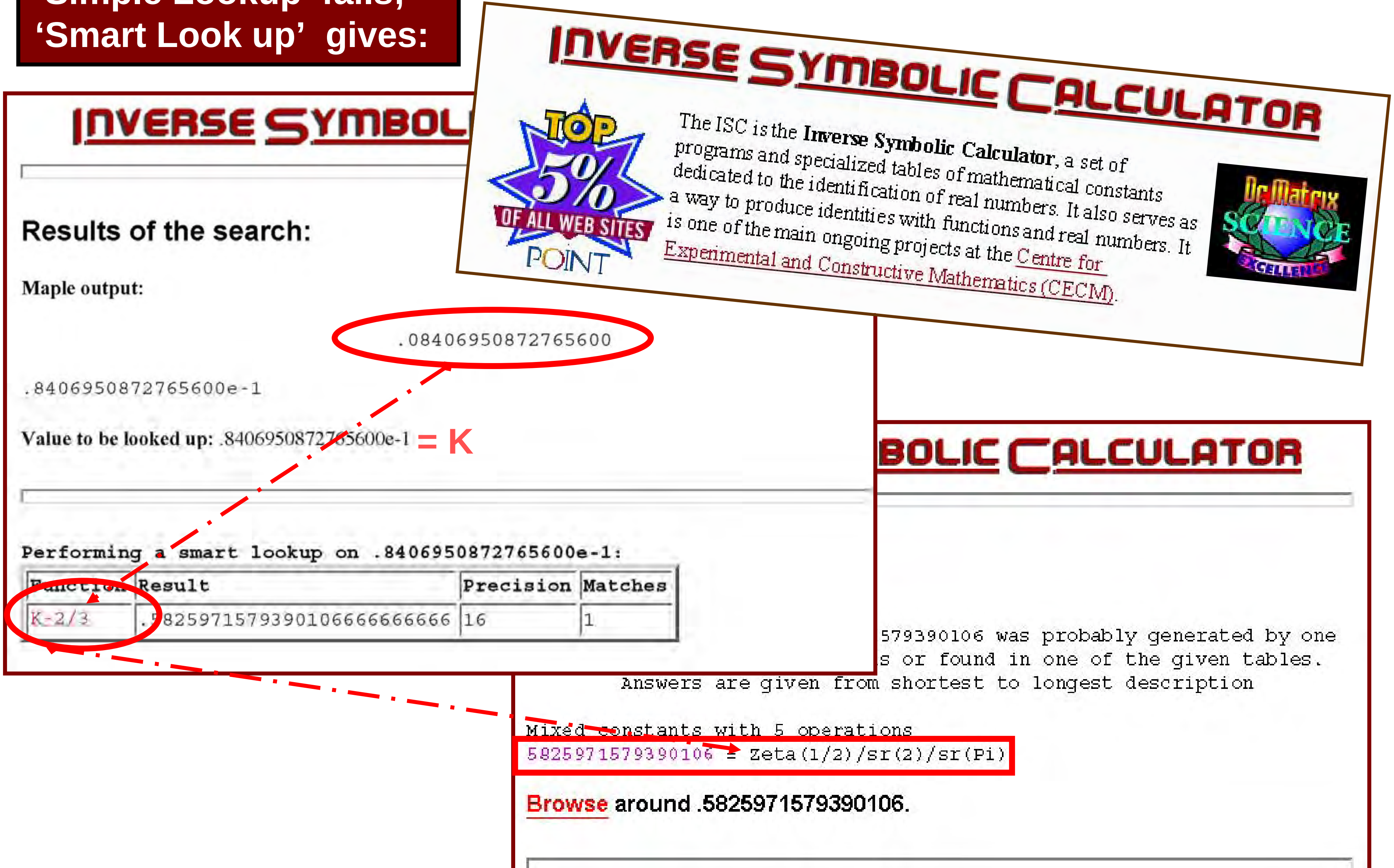
$$0.084069508727655\approx\frac{2}{3}+\frac{\zeta\,(1/2)}{\sqrt{2\,\pi}}.$$

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

ENTERING

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

‘Simple Lookup’ fails;
‘Smart Look up’ gives:



INVERSE SYMBOL

Results of the search:

Maple output:

```
.08406950872765600

.8406950872765600e-1
```

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

Performing a smart lookup on .8406950872765600e-1:

Function	Result	Precision	Matches
K-2/3	.5825971579390106666666666	16	1

INVERSE SYMBOLIC CALCULATOR

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

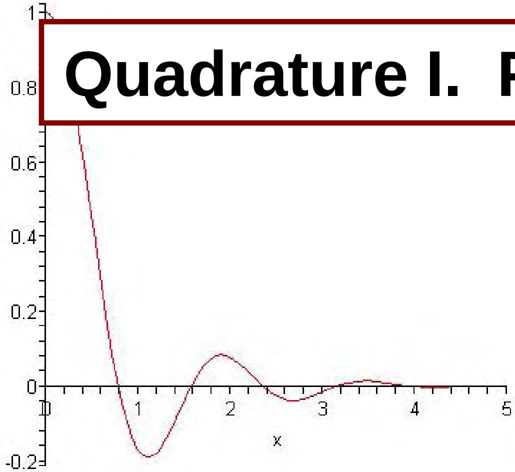
BOLIC CALCULATOR

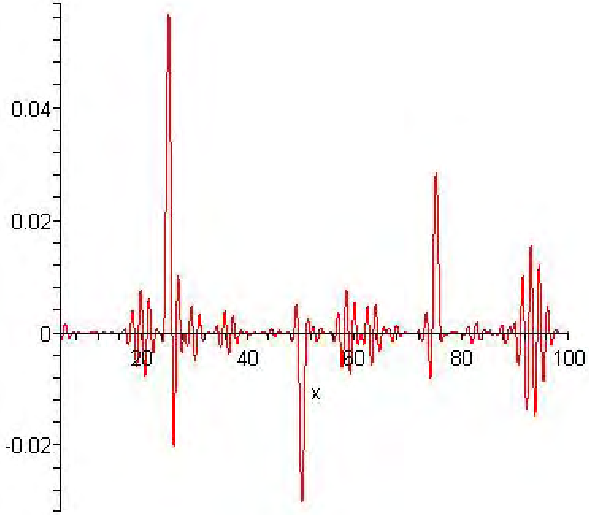
```
579390106 was probably generated by one
s or found in one of the given tables.
      Answers are given from shortest to longest description

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

Browse around .5825971579390106.

Quadrature I. Pi/8?

A numerically challenging integral





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

But π/8 is

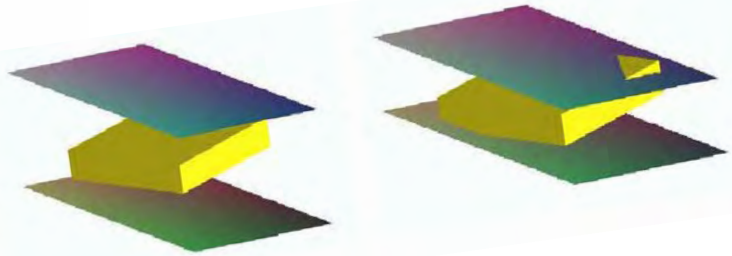
0.392699081698724154807830422909937860524645434

while the integral is

0.392699081698724154807830422909937860524646174

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

✓ Fourier analysis explains this as happening when a hyperplane meets a hypercube



Before and After

Quadrature II. Hyperbolic Knots

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

where

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

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

✓ Easiest of 998 empirical results linking physics/topology (LHS) to number theory (RHS). [JMB-Broadhurst]

We have certain knowledge without proof

Extreme Quadrature …
20,000 Digits (50 CERTIFIED)
On 1024 CPUs

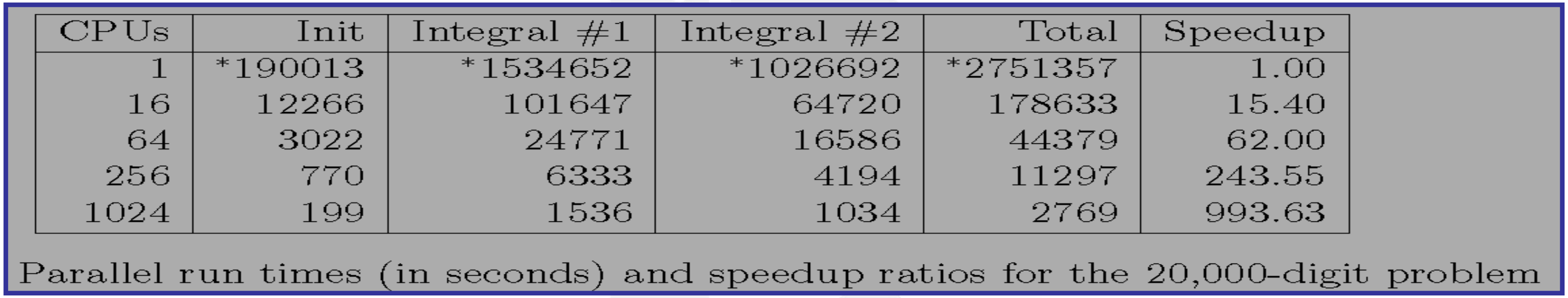
Ш. The integral was split at the nasty interior singularity

Ш. The sum was `easy’.

Ш. All fast arithmetic & function evaluation ideas used

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

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

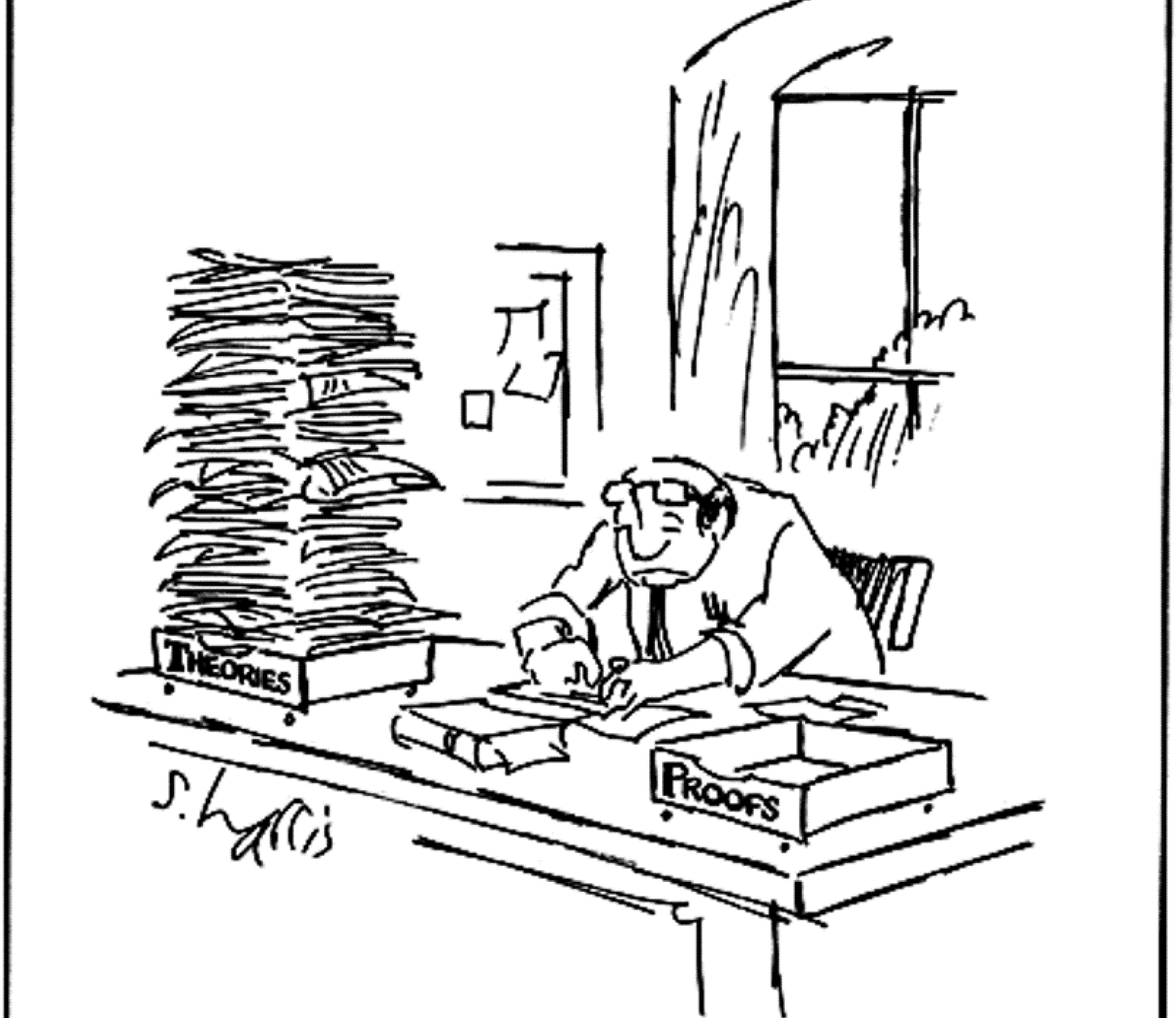


CPUs	Init	Integral #1	Integral #2	Total	Speedup
1	*190013	*1534652	*1026692	*2751357	1.00
16	12266	101647	64720	178633	15.40
64	3022	24771	16586	44379	62.00
256	770	6333	4194	11297	243.55
1024	199	1536	1034	2769	993.63

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

Expected and unexpected scientific spinoffs

- **1986-1996**. Cray used quartic-Pi to check machines in factory
- **1986**. Complex FFT sped up by factor of two
- **2002**. Kanada used hex-pi (20hrs not 300hrs to check computation)
- **2005**. Virginia Tech (this integral pushed the limits)
- **1995-** Math Resources LORs and handheld tools)


THEORIES
PROOFS
S. Harris

Outline. What is HIGH PERFORMANCE MATHEMATICS?

1. **Visual Data Mining in Mathematics.**
    - ✓ Fractals, Polynomials, Continued Fractions, Pseudospectra

2. **High Precision Mathematics.**

3. **Integer Relation Methods.**
    - ✓ Chaos, Zeta and the Riemann Hypothesis, HexPi and Normality

4. **Inverse Symbolic Computation.**
    - ✓ A problem of Knuth, $\pi/8$, Extreme Quadrature

---

5. **The Future is Here. (What is D-DRIVE?)**
    - ✓ **Examples and Issues**

6. **Conclusion.**
    - ✓ Engines of Discovery. The 21st Century Revolution
        - ✓ Long Range Plan for HPC in Canada

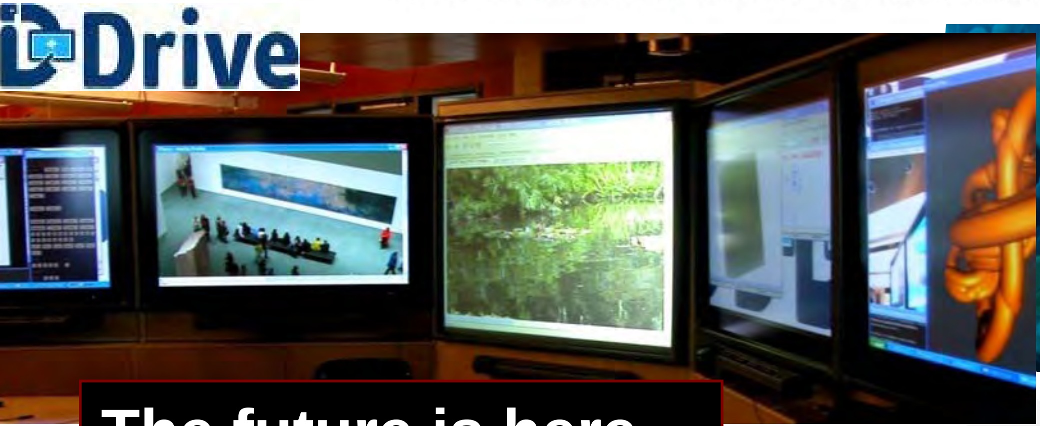
WestGrid

www.westgrid.ca

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 a.

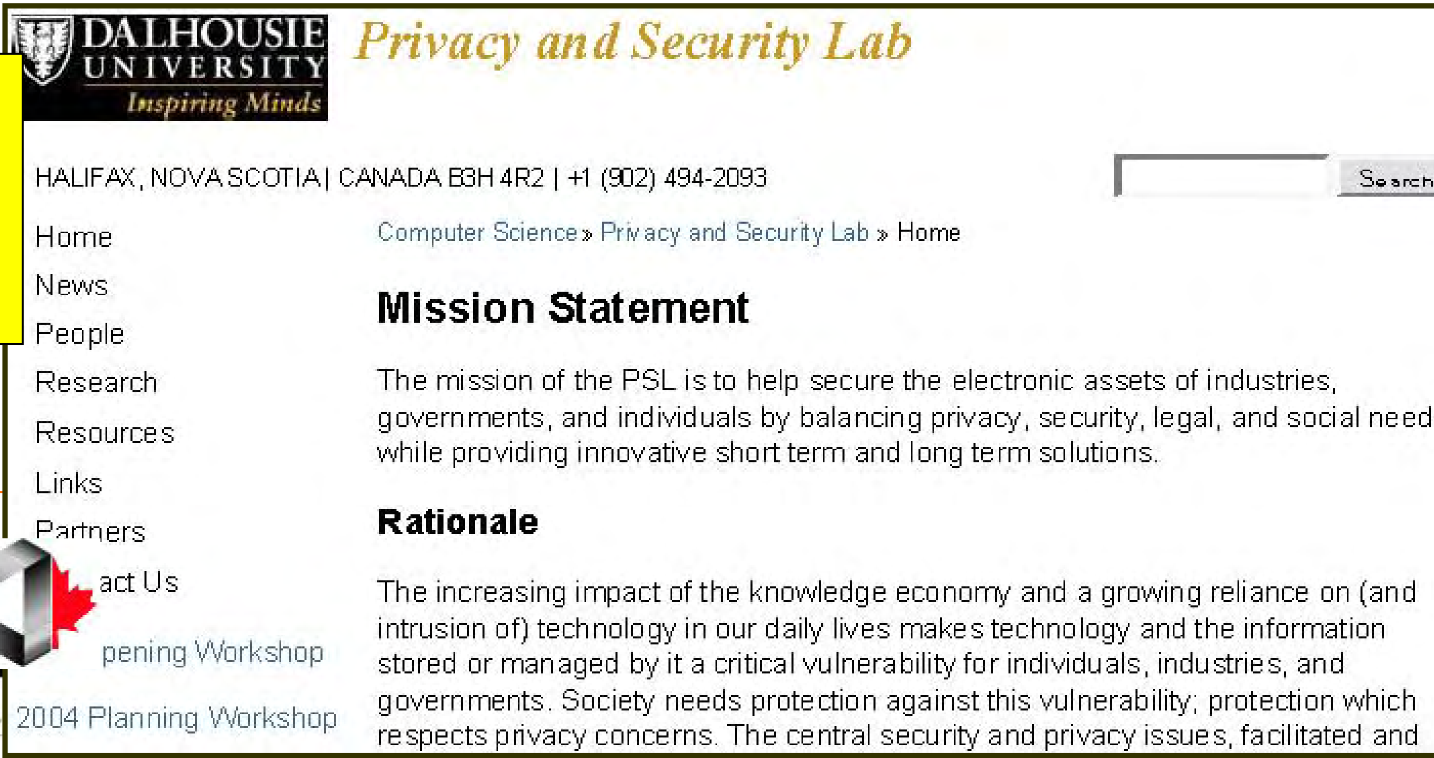
The future is here… … just not uniformly

Remote Visualization via **Access Grid**

- The touch sensitive interactive **D-DRIVE**
- An Immersive '**Cave**' Polyhedra
- and the 3D **GeoWall**

b. Advanced Knowledge Management

Projects include
- PSL
- FWDM (IMU)
- CiteSeer



DALHOUSIE UNIVERSITY *Inspiring Minds*

Privacy and Security Lab

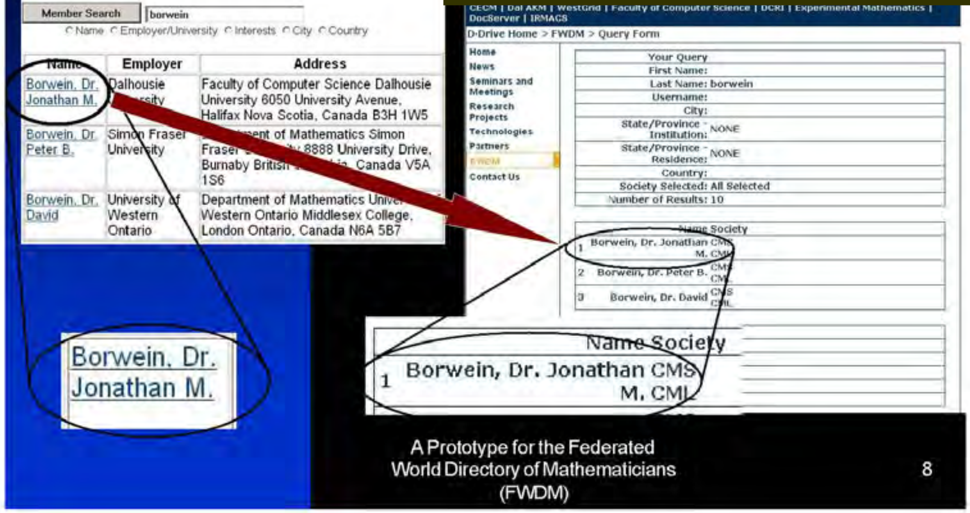
HALIFAX, NOVA SCOTIA | CANADA B3H 4R2 | +1 (902) 494-2093

Mission Statement

The mission of the PSL is to help secure the electronic assets of industries, governments, and individuals by balancing privacy, security, legal, and social need while providing innovative short term and long term solutions.

Rationale

The increasing impact of the knowledge economy and a growing reliance on (and intrusion of) technology in our daily lives makes technology and the information stored or managed by it a critical vulnerability for individuals, industries, and governments. Society needs protection against this vulnerability; protection which respects privacy concerns. The central security and privacy issues, facilitated and



Sample

CMS Canadian Mathematical Society

Name	Employer	Address
Borwein, Dr. Jonathan M.	Dalhousie University	Faculty of Computer Science Dalhousie University 6050 University Avenue, Halifax Nova Scotia, Canada B3H 1W5
Borwein, Dr. Peter B.	Simon Fraser University	ent of Mathematics Simon Fraser 8888 University Drive, Burnaby British Canada V5A 1S6
Borwein, Dr. David	University of Western Ontario	Department of Mathematics Univer Western Ontario Middlesex College, London Ontario, Canada N6A 5B7

Your Query
First Name:
Last Name: borwein
Username:
City:
State/Province - Institution: NONE
State/Province - Residence: NONE
Country:
Society Selected: All Selected
Number of Results: 10

	Name	Society
1	Borwein, Dr. Jonathan M.	CMS CML
2	Borwein, Dr. Peter B.	CMS CML
3	Borwein, Dr. David	CMS CML

Borwein, Dr. Jonathan M.

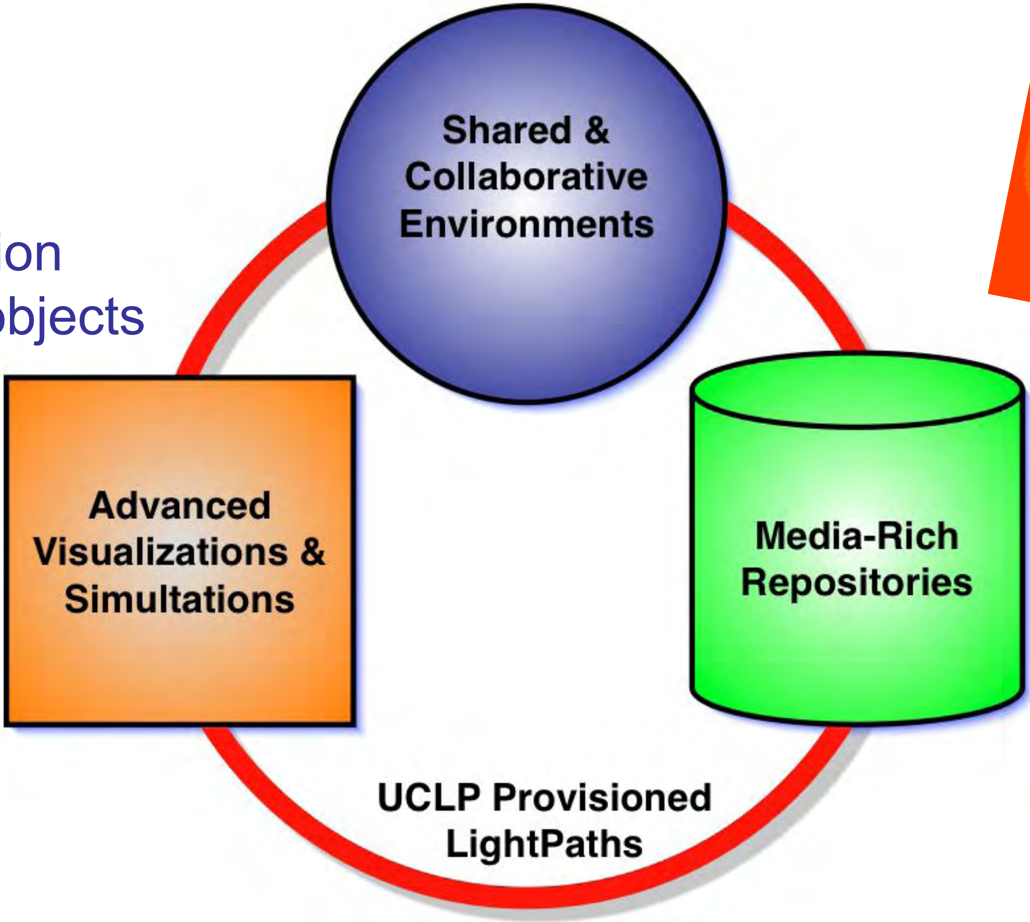
	Name	Society
1	Borwein, Dr. Jonathan M.	CMS CML

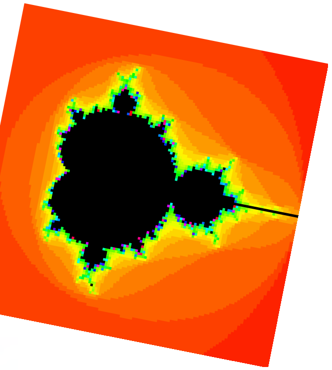
A Prototype for the Federated World Directory of Mathematicians (FWDM)

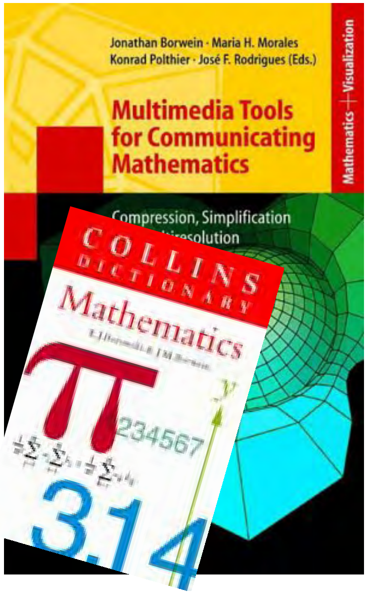
Diverse partners include
- ✓ International Mathematical Union
- ✓ CMS
- ✓ Symantec and IBM

c. Advanced Networking …

These include
- AccessGrid
- UCLP for
    - visualization
    - learning objects
    - haptics

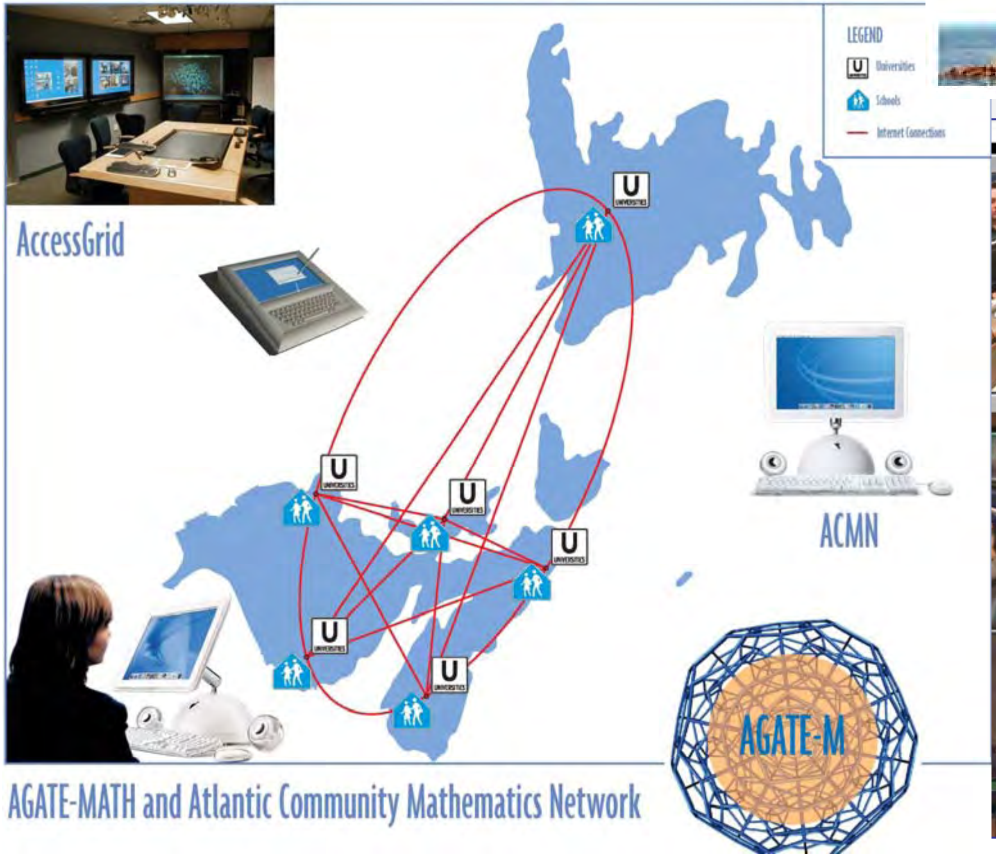




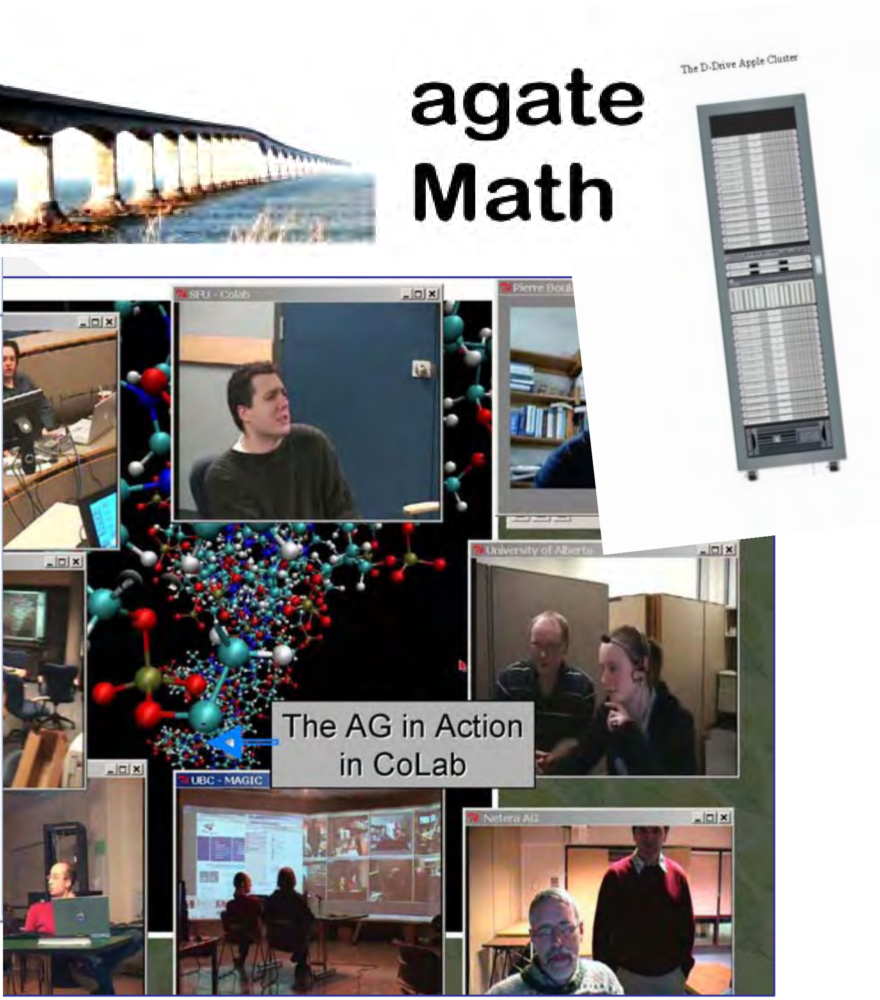


d. Access Grid, AGATE and Apple

- First 25 teachers identified



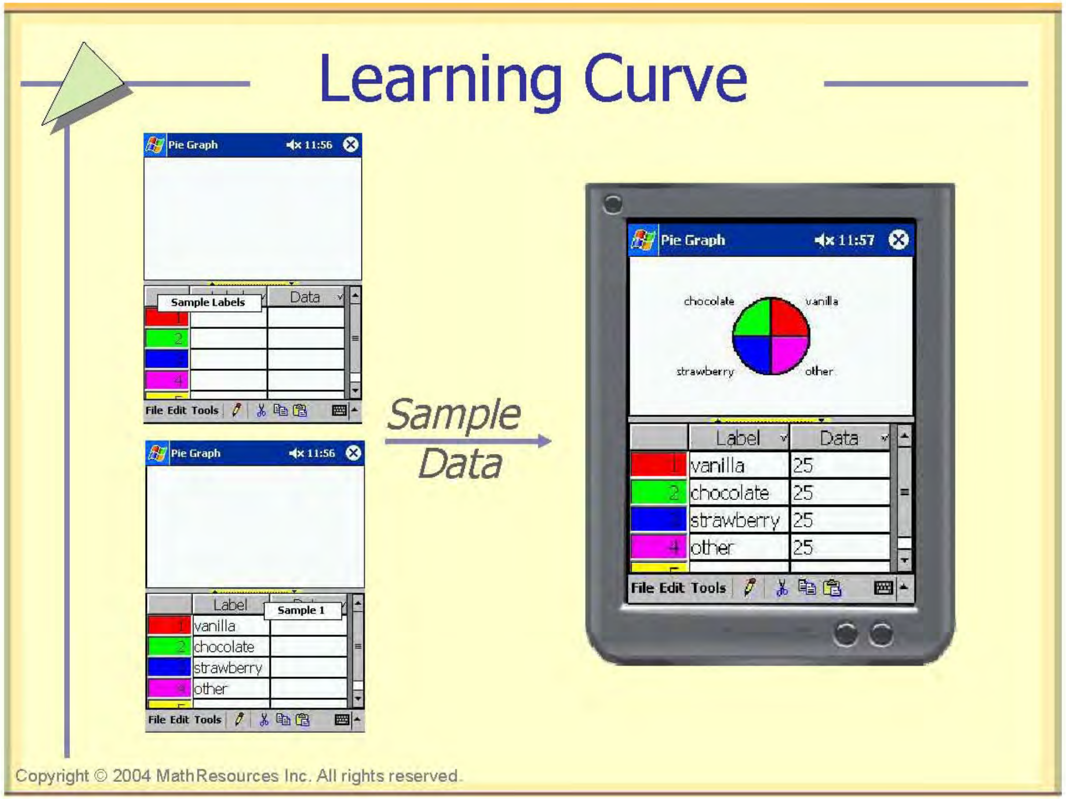
AGATE-MATH and Atlantic Community Mathematics Network



The AG in Action in CoLab

e. University – Industry links

MITACS – MRI
putting high end science
on a hand held



Learning Curve

	Label	Data
1	vanilla	25
2	chocolate	25
3	strawberry	25
4	other	25

Try your hand at new math

Firm develops software to help guide kids through maze of numbers

By **GREG MacVICAR**

Ron Fitzgerald says math is a language — and most students are illiterate.

The president of Halifax software company **MathResources Inc.** wants to change that. That's why Mr. Fitzgerald and his wife quit their jobs as book editors in Toronto in 1994.

Ten years later, he says his company … graphing calcula- … ftware for hand-

… over the next … that we can build … have $40 million … nue," Mr. Fitzger- … d-storey suite on

… fessor friends — … nd Jonathan Bor- … athResources Inc. … ted to create new … n of an interactive

… months, they spent … Mr. Fitzgerald's … e development and

… 1995 we had spent … Mr. Fitzgerald says. … ne — John Lindsay … with a line of credit

… another $300,000. … ow the chairman of … Inc.'s nine-member … ors. There are 30

… software was re- … MathResource was … gh school, college and … nts.

… thousand copies of it … ice," Mr. Fitzgerald … asn't a coup in the

… lectronic dictionaries … nd we're going to be … laughing.

… y decided to "move … nd create software for … nts. Let's Do Math: … , designed for grades 4 … sed in late 1998.

… ing respectably good … e product," Mr. Fitzger-

… eleased next year under

… r. Fitzgerald hopes will … pany really profitable in … ture is MRI-Graphing … graphing and calculating … and-held computers.

Ronald Fitzgerald, president of MathResources Inc., holds a hand-held computer capable of sh… …tion seamlessly wi… conventional computers and running the company's mathematics programs. CHRISTIAN LAFORCE

These combos will replace graphing … calcul… cause … easier …

The … **soft** W… already … Mr. Fi…

"The … He s… traditi… much s…

A pr…

… to explain technol- … says. … trying to explain … of writing notes on …

… says the graphing … ss worldwide is … dollars. He wants …

… on this project in … ery little interest … s were incredibly

… ensive," … says. … now memo- … es are big … the … faster … nd they're …

The big m… is … the U… ays, where … pick … nd-held … pute… ces so… are fo… $215 US. … way from bein… huge … ut we'll get there … Mr. Fitzger… says. "The products … too good for … not to get there

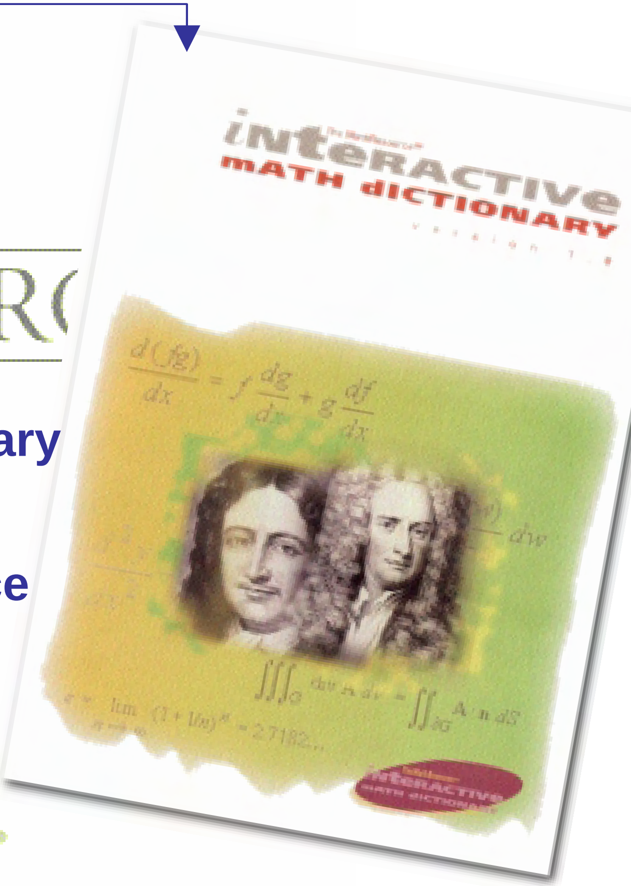
mitacs

MathResources Inc.

MRI’s First Product in Mid-nineties

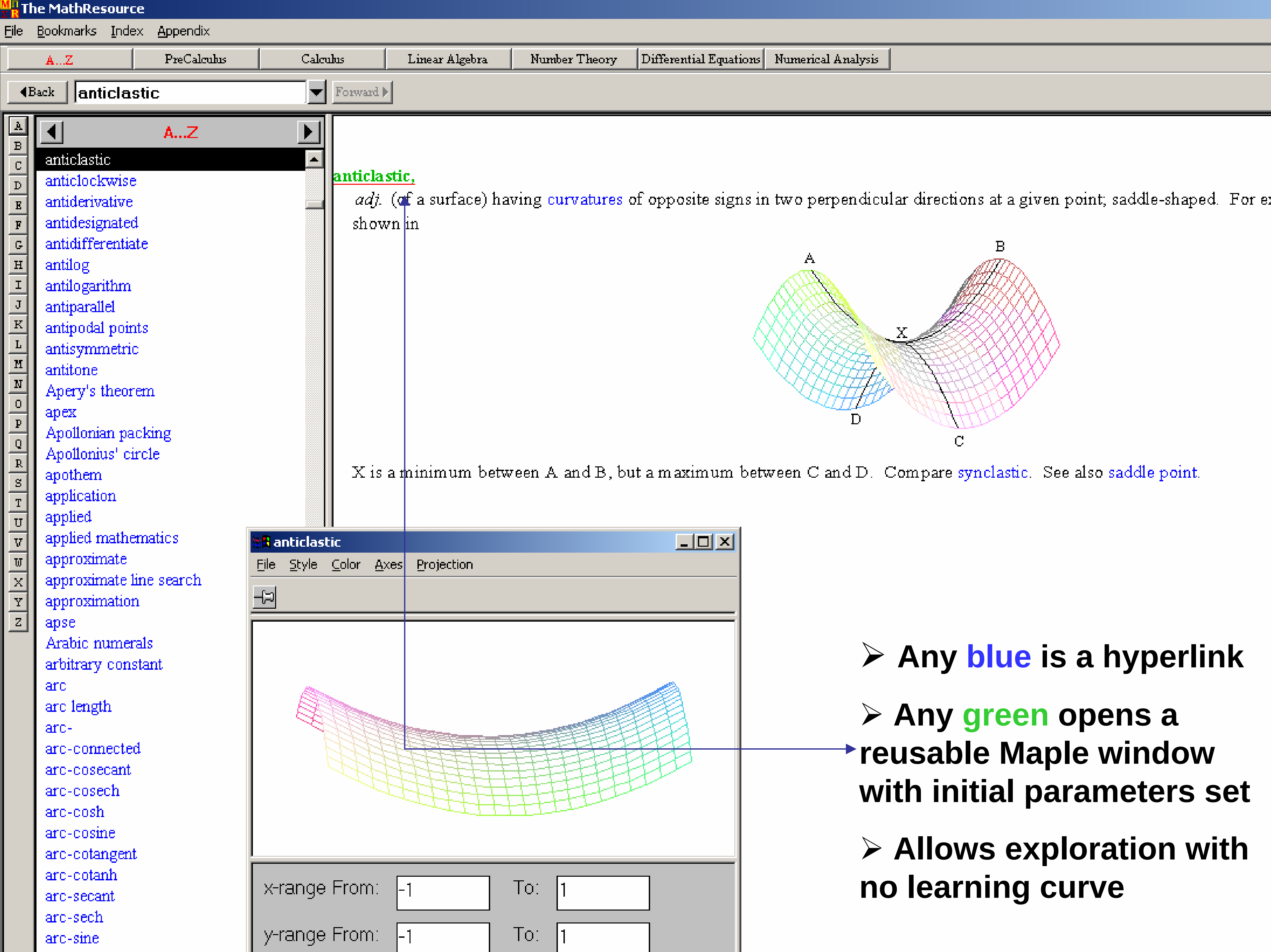
THE HARPER COLLINS DICTIONARY
MATHEMATICS
In-Depth Explanations and Examples Covering Over 4,000 Entries with Extensive Diagrams and Charts
E.J. Borowski & J.M. Borwein

Maplesoft



interactive
MATH dictionary

- ▶Built on **Harper Collins dictionary** - an IP adventure!
- ▶ **Maple** inside the **MathResource**
- ▶ **Data base** now in **Maple 9.5**
- ▶ **CONVERGENCE?**



anticlastic,

adj. (of a surface) having curvatures of opposite signs in two perpendicular directions at a given point; saddle-shaped. For ex

shown in

X is a minimum between A and B, but a maximum between C and D. Compare synclastic. See also saddle point.

x-range From: -1 To: 1

y-range From: -1 To: 1

- **Any blue is a hyperlink**
- **Any green opens a reusable Maple window with initial parameters set**
- **Allows exploration with no learning curve**

Outline. What is HIGH PERFORMANCE MATHEMATICS?

1. Visual Data Mining in Mathematics.
   - ✓ Fractals, Polynomials, Continued Fractions, Pseudospectra
2. High Precision Mathematics.
3. Integer Relation Methods.
   - ✓ Chaos, Zeta and the Riemann Hypothesis, HexPi and Normality
4. Inverse Symbolic Computation.
   - ✓ A problem of Knuth, $\pi/8$, Extreme Quadrature
5. The Future is Here.
   - ✓ Examples and Issues
6. Conclusion.
   - ✓ Engines of Discovery. The 21st Century Revolution
     - ✓ Long Range Plan for HPC in Canada

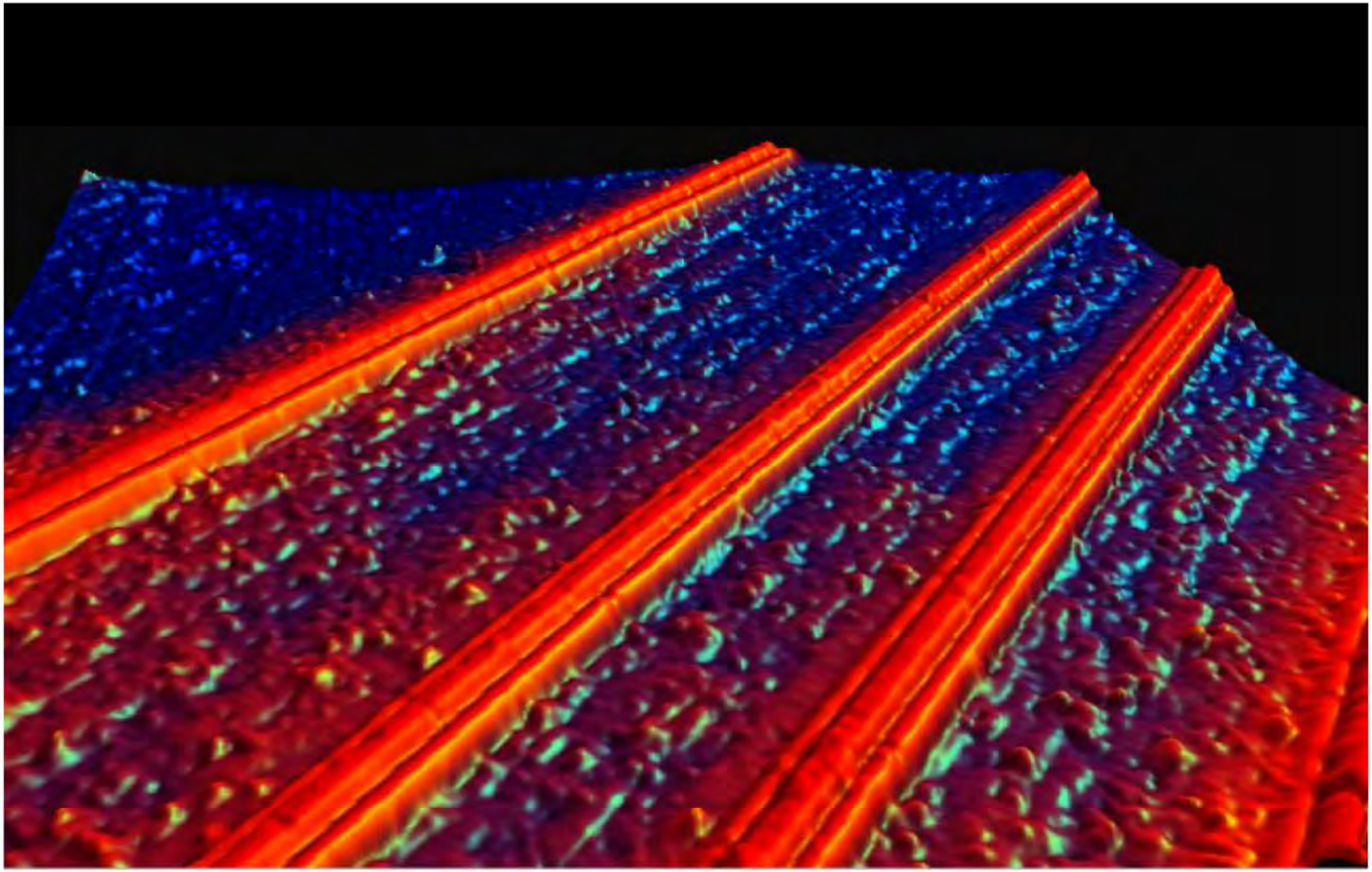
CONCLUSION

ENGINES OF DISCOVERY: The 21st Century Revolution

The Long Range Plan for High Performance Computing in Canada

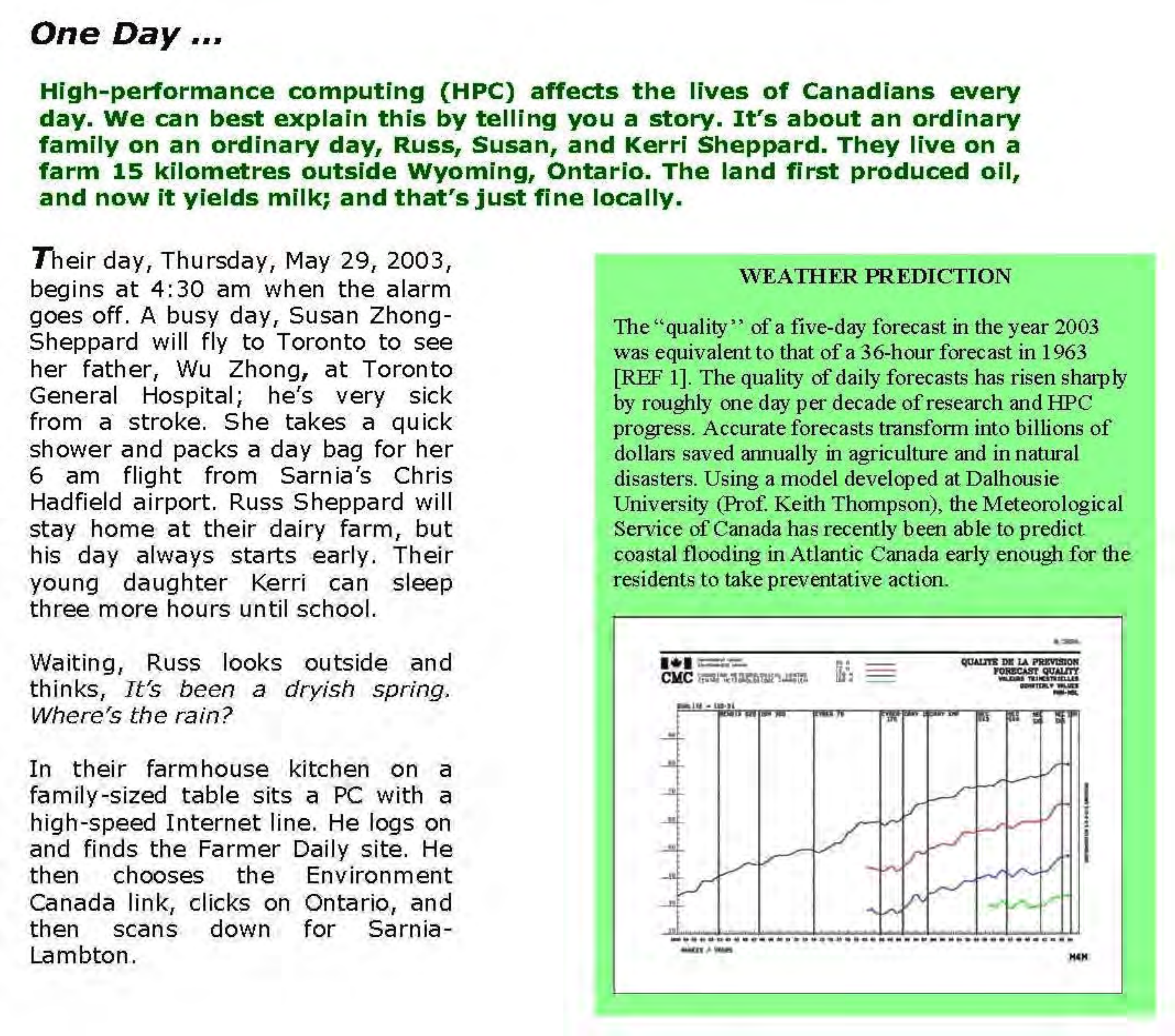
Self-Assembled Wires 2nm Wide

[P. Kuekes, S. Williams, HP Labs]



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.

The backbone that makes so much of our individual science possible

WWW.C3.CA

Enabling Canadian research excellence through high performance computing

Favoriser l'excellence en recherche au Canada avec le calcul de haute performance

REFERENCES


Enigma

J.M. Borwein and D.H. Bailey, *Mathematics by Experiment: Plausible Reasoning in the 21st Century* A.K. Peters, 2003.

J.M. Borwein, D.H. Bailey and R. Girgensohn, *Experimentation in Mathematics: Computational Paths to Discovery,* A.K. Peters, 2004.

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

> *“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.