Experimental Mathematics: Computational Paths to Discovery



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

"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?



Revised15/06/2005



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

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
 - $\checkmark~$ Long Range Plan for HPC in Canada





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

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, infnite 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 Crundall, 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 simplified is raising unsettling questions about how to regard experimental results

"I have some of the excitement that Leonardo of Pisa must have felt when he encountered Arabic arithmetic. It suddenly made certain calculations flabbergastingly easy," Borwein says. "That's what I think is happening with computer experimentation today," EXPERIMENTERS OF OLD 2.

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 low 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 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-



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

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



IBM BlueGene/L system at LLNL

System (64 cabinets, 64x32x32)

180/360 TF/s

16 TB DDR

Cabinet (32 Node boards, 8x8x16)

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

Compute Card (2 chips, 2x1x1)

Chip (2 processors)

90/180 GF/s 8 GB DDR

2.8/5.6 GF/s 4 MB 5.6/11.2 GF/s 0.5 GB DDR

217 cpu's

2.9/5.7 TF/s 256 GB DDR

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



Grand Challenges in Mathematics (CISE 2000)

Are few and far between

- Four Colour Theorem (1976,1997)
- Kepler's problem (Hales, 2004-10)
 next 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?
- 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

Fano plane of order 2

An Inadmissible Two-Colouring



- 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



5 SMART Touch-sensitive Interwoven Screens

Drive

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

About the Cover

Extreme 3D visualization

The background image of this month's cover is a photograph included by Jonathan Borwein and David Bailey, perhaps somewhat whimsically. in their article on experimental mathematics. The photograph was taken for a publicity brochure for the now defunct New Media Innovation Centre in downtown Vancouver, British Columbia, an organization partially sponsored by Simon Fraser University, to which Borwein is affiliated. The two young men, who are graduate students in the the department of Electrical and Computer Engineering at the University of British Columbia, are in a kind of box with what might be called surround-projection. The approximate spheres are displayed in duplicate at rapidly alternating times in synchronization with the goggles they are wearing, so that what they see is a simulated 3D image, not just the flat projections on the walls on their box. The projections are interactive, controlled by input through a key pad held by Timothy Chen, the student on the right. The project the students are involved in is part of Mr. Chen's studentwork at U. B. C. What is being projected is a flow field of spheres in a cylinder with various obstacles interactively superimposed into the flow. The inset photographs are screen displays produced by Mr. Chen from the same project.

It's hard to imagine exactly what role such high end visualization technology will play in mathematical research, but not impossible. One likely application for similar, but not quite so sophisticated, display systems might very well be in public presentations. The effects can be spectacular.

Brian Corrie of Simon Fraser University provided us with the digital version of the background photograph.

-Bill Casselman, Graphics Editor (notices-cover@ams.org)



May 2005 AMS Notices Cover





Dalhousie Distributed Research Institute and Virtual Environment

East meets West: Collaboration goes National

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

- High Performance Computing
- Mathematical and Computational Science Research
- Science Outreach
 - ✓ Educational
 - ✓ Research



Centre seen as 'serious nirvana'

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

The 2,500 square metre IRMACS research centre

 \checkmark The building is a also a 190cpu G5 Grid

✓ At the official April opening, I gave one The \$14 million centre's of the four presentations from **D-DRIVE**

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.

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 terina research s whose is the computer. Trans-Canada Seminar Thursdays PST 11.30 MST 12.30 AST 3.30



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.

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 dustering technology, designed at SFU, and sees a to West Originan ultra high second interpretingial activaly with shared accounting and exclaimed in



Mathematical Data Mining

Experimentation

Mathematics

Computational Paths to Discovery

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)

n Barwein

vid Bailey Roland Girgensohn

athematics BENPERIMENT

Jonathan Borwein

David Bailey

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

INDRA'S PEARLS The Vision of Felix Klein

David Mumford, Caroline Series, David Wright





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



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.

- <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 THREE SCALES

Pictures are more democratic but they come from formulae

Roots in the most stable colouring



HE FRONTIERS COLLECTION

J. G. Roederer

INFORMATION AND ITS ROLE IN NATURE





Ramanujan's Arithmetic-Geometric Continued fraction (CF)





A cardioid

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

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

 \Box 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?

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



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





'Large' (10⁵ to 10⁸) Matrices must be seen

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



A dense inverse



Pseudospectrum of a banded matrix

The ε-pseudospectrum of A

- is: $\sigma_{\varepsilon}(A) = \{x : \exists \lambda \text{ s.t. } \|Ax \lambda x\| \le \varepsilon\}$
 - \checkmark for ε = 0 we recover the eigenvalues

 \checkmark full pseudospectrum carries much more information

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

Rob Scharein's KnotPlot

Visualization

Perko pair knots

These are the famous Perko pair knots, listed as distinct knots in many knot tables since the 19th century, until Kenneth Perko showed in 1974 that they were in fact the same knot. He proved the equivalence by showing a sequence of diagrams leading from one to the other. The following sequence is a different demonstration of the same fact, obtained by relaxing the two knots using <u>KnotPlot</u>.

A movie of the deformation is included as one of the standard KnotPlot demos. View it by first <u>installing</u> <u>KnotPlot</u>, then dick on the "DemoA" panel and then "Perko pair".

Perko A (10161)

Perko B (10₁₆₂)











Dalhousie Distributed Research Institute and Virtual Environment



C3 Membership

Haptics in the MLP

Haptic Devices extend the world of I/O into the tangible and tactile





We aim to link multiple devices together such that two or more users may interact at a distance

- in Museums and elsewhere
- Kinesiology, HCI

Sensable's Phantom Omni

SensAble

MEDIALIGHTPATHS

And what they do



Force feedback informs the user of his virtual environment adding an increased depth to human computer interaction





The user feels the contours of the virtual die via resistance from the arm of the device

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

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A WARMUP Computational 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.



 $|P(\alpha)| > -$

QED

Likewise, suppose we know α is algebraic of degree d and length I (coefficient sum in absolute value)

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



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

Proof. Purely **qualitative analysis** with partial fractions and arctans shows integral is $\pi \beta$ where β is algebraic of degree *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**: $||\beta - 1| < 1/(32L) \mapsto \beta =$

✓ A fully symbolic Maple proof followed.

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



Parallel derivative free optimization in Maple



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 <u>Welcome</u> 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

Maple on SFU 192 cpu `bugaboo' cluster

- different node sets are in different colors



Greetings from the On-Line Encyclopedia of Integer Sequences!

ATAT 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)]

An Exemplary Database

ID Number: A000055 (Formerly M0791 and N0299) URL : http://www.research.att.com/projects/OEIS?Anum=A000055 1, 1, 1, 1, 2, 3, 6, 11, 23, 47, 106, 235, 551, 1301, 3159, 7741, 19320, Sequence: 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.
- P. J. Cameron, Sequences realized by oligomorphic permutation groups J. Integ. Seqs. Vol Links: Steven Fingh, 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. 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-tree

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

Integrated real time use moderated

- 100,000 entries

- grows daily

- AP book had 5,000







Fast Arithmetic (Complexity Reduction in Action)

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

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
- Elementary and special functions
 - ✓ via Elliptic integrals and Gauss AGM

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!



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



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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 α is algebraic of degree N, consider $(1, \alpha, \alpha^2, ..., \alpha^N)$

Peter Borwein in front of Helaman Ferguson's work

> CMS Meeting December 2003 SFU Harbour Centre

Ferguson uses high tech tools and micro engineering at NIST to build monumental math sculptures





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



Wilf-Zeilberger Algorithm Drive

is a form of automated telescoping:

$$\sum_{n=1}^{\infty} \frac{1}{n(n+1)} = \sum_{n=1}^{\infty} \left\{ \frac{1}{n} - \frac{1}{n+1} \right\} = 1$$

✓ AMS Steele Research Prize winner. In Maple 9.5 set:

$$F := \frac{(3\,n+k-1)!\,(n+k)!\,(-n+k-1)!\,(2\,n)!\,(n-1/2)!\,\left(1/4\right)^k}{(3\,n-1)!\,n!\,(-n-1)!\,(2\,n+k)!\,(n-1/2+k)!\,k!}, \quad r := \frac{\binom{2\,n}{n}}{\binom{3\,n}{n}}$$

and execute:

- > with(SumTools[Hypergeometric]):
- > WZMethod(F,r,n,k,'certify'): certify;

which returns the certificate

/ 2
$$\$$

\11 n + 1 + 6 n + k + 5 k n/ k
3 (n - k + 1) (2 n + k + 1) n

This proves that summing F(n,k) over k produces r(n), as asserted.



Dalhousie Distributed Research Institute and Virtual Environment

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

<u>Abstract of the future</u> 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.

"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 When das Anyakt der Prinnyalles under as 'Paper of the Millennium'? Jegebones Groces. (Badene horabbindle, 1859, Normalin) RH is so here Dans findre Angeiling, wells une der her important dente durch der Aufrahme unter ihr Corresponbecause it de shen hat you That and have a glande ich and back vields precise detunes to excern tight, dass is rander hidrich results on estalline Estantino baldings getrand machinder distribution and Arther les eres bet rendeng abor de die figent behaviour of der Primzahle; ein Gegenden, wilder dires des primes Assesse, aller Games and Diviceles demaile langere fit good with hale, and colden hiteraling viele well will go y works and int. their dieser lector and good on is als Anyeng pund die von Ealer gemache Bemerring, Von De Produes Euler's product makes the key link $\mathcal{T} - \frac{1}{1 - \frac{1$ between Primes and ζ was fir pelle Prompalle, fir malle garro Tall



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)

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





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

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



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

- 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

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;



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/	• © (G-	345
Getting Started Latest Headline	s 就 www.icbc.ca			
PiHex ha	The The	to calculate Pi. 2 Quadrillionth Bit of P Forty Trillionth Bit of P Five Trillionth Bit of P iject which used idle computing power to set th	' <u>i is '0'!</u> Pi is '0'! Pi is '0'!	ercival 2004 which is a specific bits of Pi.
hits since the counter last reset.	Position	Hex Digits Beginnin At This Positic	-	
Undergraduate Colin Percival's grid computation PiHex rivaled Finding Nemo	$10^{6} \\ 10^{7} \\ 10^{8} \\ 10^{9} \\ 10^{10} \\ 10^{11} \\ 1.25 \times 10^{12} \\ 2.5 \times 10^{14}$	26C65E52CB459 17AF5863EFED8 ECB840E219261 85895585A0428 921C73C6838F1 9C381872D2759 07E45733CC790 E6216B069CB60	OB	on 1736 PCS countries 2 million Cpu-hours

PSLQ and Normality of Digits



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

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

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

Consider the hex digit stream:

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

 \checkmark We have checked that this gives first million hex-digits of Pi.

✓ <u>Is this always the case</u>? The weak Law of Large Numbers implies this is very probably true!

Pi to 1.5 trillion
places in 20 steps
This fourth order
algorithm was
used on all big-
$$\pi$$

computations from
1986 to 2001
$$y_{a} = \frac{1 - (1 - y_{k}^{4})^{1/4}}{1 + (1 - y_{k}^{4})^{1/4}}$$
 and
 $a_{k+1} = a_{k}(1 + y_{k+1})^{4}$
 $= \frac{1 - (1 - y_{k}^{4})^{1/4}}{1 + (1 - y_{k}^{4})^{1/4}}$ and
 $a_{k+1} = a_{k}(1 + y_{k+1})^{4}$
 $= 2^{2k+3}y_{k+1}(1 + y_{k+1})^{4}$
Then $1/a_{k}$ converges quartically to π
 $x = \frac{1 - (1 - y_{k}^{4})^{1/4}}{1 + (1 - y_{k}^{4})^{1/4}}$ and
 $a_{random walk on a$

A random walk on a million digits of Pi



IF THERE WERE COMPUTERS IN GALILEOS TIME

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An Inverse and a Color Calculator



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



id	entify(sqrt(2	.)+sqrt(3.))	
		$\sqrt{2}$	$+\sqrt{3}$	

INVERSE SYMBOLIC CALCULATOR

Please enter a number or a Maple expression:	Clear
O <u>Simple Lookup and Browser</u> for any number. O <u>Smart Lookup</u> for any number.	
 <u>Generalized Expansions</u> for real numbers of at least 16 digits. <u>Integer Relation Algorithms</u> for any number. 	
▲ ? , :	

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 – 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

 $W \exp(W) = x$



surface

Donald Knuth* asked for a closed form evaluation of:

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

- 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)





But $\pi/8$ is

<u>0.39269908169872415480783042290993786052464</u>5434

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



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

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

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

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



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

Γ	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 (next overhead)



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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**
- An Immersive 'Cave'
 Polyhedra
- and the 3D GeoWall

... just not uniformly



a. ACENet and HPC@DAL



WestGrid

Dalhousie Distributed Researc

ACEnet completes the Pan Canadian Consortia



CLUMEQ

HPCVL

SHARCNET

Enabling Canadian Favoris research excellence en rech through high avec le erformance computing de hau



ACENER

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

b. Advanced Knowledge Management



Search



c. Advanced Networking ...

Dalhousie Distributed Research Institute and Virtual Environment

Drive



Haptics in the MLP

SensAble

Haptic Devices extend the world of I/O into the tangible



We aim to link multiple devices together such that two or more users may interact at a distance

• in Museums and elsewhere

and tactile

Sensable's Phantom Omni

What these Haptic devices do





 Force feedback informs the user of his virtual environment adding an increased depth to human computer interaction





 The user feels the contours of the virtual die via resistance from the arm of the device
d. Access Grid, AGATE and Apple

Dalhousie Distributed Research Institute and Virtual Environment

Drive

First 25 teachers identified



agate Atlantic Gateway to Mathematics

AGATE-MATH was recently established for the purpose of improving, encouraging, and supporting the teaching of mathematical sciences, in Atlantic Canada and elsewhere.

Vision Statement

The discipline of Mathematics is beautiful and important in its own right. At the same time mathematics and mathematical competency are critical to most other scientific disciplines and are pervasive in modern society. Cell phones, Google, e-banking, internet security, "Finding Nemo," all use enormously sophisticated mathematics, as do countless more obvious examples from medical imaging to mutual funds.

Mathematics is a fundamental component of the language of science. Consequently, mastery of basic mathematics is critical for sustaining interest not only in the pursuit of science but also in understanding the sciences (physical, biological, artificial, social and human) that affect our lives. Successful scientists and engineers typically report a serious early engagement with mathematics as one of their formative experiences. Base competency and interest in mathematics and science are often achieved or lost before the end of high school and likely by the end of elementary grades.

Goals of AGATE-M

- To create a network linking everyone with an interest in math education.
- To enable easy communication between teachers and researchers.
- To strengthen the sense of community amongst those who share the goal of improving math education.
- To provide a forum for the discussion of current issues.
- To offer enrichment resources through web based resources.
 - To facilitate the dissemination of knowledge and experience.

To stimulate enthusiasm and creative thinking in our community.

e. University – Industry links

MITACS – MRI

putting high end science

on a hand held

BUSINESS

Wednesday, December 15, 2004 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 company matheestarces inc. wants to and his wife quit their jobs as book editors in Toronto in 1994 Ten years later, he says his compar-

raphing calculaftware for hand

> over the nex that we can build have \$40 million ue," Mr. Fitzgerd-storey suite on

fessor friends id 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. now the chairman of inc.'s nine-member ors. There are 30

software was re-MathResource was th school, college and

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 He s traditie much s graphing and calculating A pro and held computers.

calcul

ca1150

easier

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soft W

alread Mr. Fit

"Th



eventional computers and running the company's mathema to explain technol will re



were incredibly



Par Martin

seamlessly

ery little interest



INCONACTIVO MATH ALCTIONARY



MathResources Inc.



Copyright © 2004 Math Resources Inc. All rights reserved

MRI's First Product in Mid-nineties PAVCA SED MATVRA





MATHRESOUR

Built on Harper Collins dictionary - an IP adventure!

- Maple inside the MathResource
- Data base now in Maple 9.5

► CONVERGENCE? athResources Inc.

*** surface	- O ×	surface
Eile Style Color Axes Projection		Elle Style Color Axes Projection
-		
A plot of		The surface
$r = 1.3^t \sin(p)$		$z = \sin(x) + \cos(y)$
in spherical coordinates		
		x-range From: 0 To: 2*Pi
		y-range From: 0 To: 2*Pi
		Plot Reset
	1	
		Elle Style Color Axes Projection
theta (t) range From: -1 To:	2*Pi	theta (t) range From: -15*cos(2* To: 10*cos(3*t)
	2 11	
phi (p) range From: 0 To:	Pi	z-range From 4 To: 0
	-	



Building on products such as:

MRI Graphing Calculator & Robert Morris College

Ed Clark, an instructor at Robert Morris College, has been using the MRI Graphing Calculator with his students. Ed says:

- "The learning curve for the MRI Graphing Calculator is very very short."

"Just the fact that a handheld computer" displays color is huge."



Graphing in Color-



Traditional Graphing Calculator



Learning Curve



A selection of appropriate virtual manipulables



-

Index

💙 Parabola Paradox Parallel Parallelogram Parameter Parametric equation Parentheses Partial product of an infinite product Partial sum of an infinite series >> Pascal's triangle Pascal, Blaise > Peg game Pentagon Sentagonal number Percent ▶ Percentage change

- Percentage decrease
 Percentage increase
 Percentile
 Perfect number
 Perfect square
 Perfect square trinomial
 Perimeter
- >> Period of a function
- Permutation
 Perpendicular
 Perpendicular bisector
 Phase shift
 - Pi Pick's formula
- Pictograph
 Pie graph
 Pint
 Place value
 Plane
 Plane figure
 - Plane of symmetry
 - Plane symmetry

Platonic solids

Also called regular polyhedra.

The five special <u>polyhedra</u> where all of the <u>faces</u> of each polyhedron are <u>congruent</u> regular polygons and the same number of polygons meet at each <u>vertex</u>. The ancient Greeks proved that there are only five platonic solids. They are: <u>cube</u>, <u>tetrahedron</u>, <u>octahedron</u>, <u>dodecahedron</u>, and <u>icosahedron</u>.

Click on one of the polyhedra below and drag the mouse to rotate it. By right clicking on one of the polyhedra you can change to a wire frame view.



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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

HOP

Budget

Technology

Operations

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.



25 Case Studies many sidebars





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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.