Experimental Mathematics: Computational Paths to Discovery



Dalhousie Distributed Research Institute and Virtual Environment



What is HIGH PERFORMANCE MATHEMATICS?

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"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?



Revised 11/5/05

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



This picture is worth 100,000 ENIACs



Indra's Pearls A merging of 19th and 21st Centuries

INDRA'S PEARLS The Vision of Felix Klein

David Mumford, Caroline Series, David Wright





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

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-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

- 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

DDRIVE's Five 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



Mathematical Data Mining

Experimentation Mathematics

Computational Paths to Discovery

a Borwein

lavid Bailey

An unusual Mandelbrot parameterization

Three visual examples follow

✓ Roots of `zero-one' polynomials ✓ Ramanujan's continued fraction ✓ Sparsity and Pseudospectra

Roland Girgensolin AK Peters, 2004 (CD in press)

athematics HEHPERIMENT

Jonathan Borwein

David Bailey



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



and in the most stable colouring



J. G. Roederer

INFORMATION AND ITS ROLE IN NATURE

Deringer





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

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

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

 \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?



Mathematics and the aesthetic Modern approaches to an ancient affinity

(CMS-Springer, 2005)



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

> Oliver Heaviside (1850 - 1925)

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





Pseudospectra or Stabilizing Eigenvalues

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

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

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



A dense inverse





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)



An infinite dimensional integral equation in laser theory
 ✓ discretized to a matrix of dimension 600
 ✓ projected onto a well chosen invariant subspace of dimension 109

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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

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 mathenatical 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 [mathematician] field has been transformed by it," says Richard Crundall, a mathematician at Reed Collego in Portland, Ore. "Instead of just being a number-encoding 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 is raising unsettling questions about how to regard experimental results

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

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

For instance, in 1666, sheer curiosity and love of numbers led Isaac. Newton to calculate directly the first 16 digits of the number pi, later writing, "I arn 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-cent

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 too one of the most important conjectures in the history of number theory: that the mumber of prime numbers less than a number x is roughly equal to x divided by the locarithm of a.

divided by the logarithm of *n*. 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

A WARMUP Computational Proof

> Suppose we know that $1 < \alpha < 10$ 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.



 \succ 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



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

QED

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

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

✓ 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



 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 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 the SFU 192 cpu cluster

- different node sets are in different colors



Greetings from the On-Line Encyclopedia of Integer Sequences!

Lookup | Index | Browse | Format | Contribute | EIS | NJAS

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: <u>A000055</u> (Formerly M0791 and N0299) URL: http://www.research.att.com/projects/OEIS?Anum=A000055 Sequence: 1,1,1,1,2,3,6,11,23,47,106,235,551,1301,3159,7741,19320, 48629,123867,317955,823065,2144505,5623756,14828074, 39299897,104636890,279793450,751065460,2023443032, 5469566585,14830871802,40330829030,109972410221

Name: Number of trees with n unlabeled nodes.

- Comments: Also, number of unlabeled 2-gonal 2-trees with n 2-gons.
- References F. Bergeron, G. Labelle and P. Leroux, Combinatorial Species and Tree-Like Structures, Camb. 1998, p. 279.
 - N. L. Biggs et al., Graph Theory 1736-1936, Oxford, 1976, p. 49.
 - S. R. Finch, Mathematical Constants, Cambridge, 2003, pp. 295-316.

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

- F. Harary, Graph Theory. Addison-Wesley, Reading, MA, 1969, p. 232.
- F. Harary and E. M. Palmer, Graphical Enumeration, Academic Press, NY, 1973, p. 58 and 244.
- D. E. Knuth, Fundamental Algorithms, 3d Ed. 1997, pp. 386-88.
- R. C. Read and R. J. Milson, An Atlas of Graphs, Oxford, 1998.
- J. Riordan, An Introduction to Combinatorial Analysis, Wiley, 1958, p. 138.
- Links: P. J. Cameron, Sequences realized by oligomorphic permutation groups J. Integ. Seqs. Vol. Steven Finon, Otter's Tree Enumeration Constants
 - E. M. Rains and N. J. A. Sloane, On Cayley's Enumeration of Alkanes (or 4-Valent Trees), J
 - 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.: $\lambda(x) = 1 + T(x) - T^2(x)/2 + T(x^2)/2$, where $T(x) = x + x^2 + 2^{\pm}x^3 + ...$







Fast Arithmetic (Complexity Reduction in Action)

Multiplication

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

- $\checkmark\,$ in ranges from 100 to 1,000,000,000,000 digits
- The other operations
 - ✓ via Newton's method

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

- Elementary and special functions
 - $\checkmark\,$ via Elliptic integrals and the Gaussian 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

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



Drive

- 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

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 Prinzallen under as 'Paper of the Millennium'? Jegilines grine. (Badene horable sidle, 1859, Non mber?) RH is so here Dans firder Angridany, wells wer das her important dente dures der Aufreisen under ihre Conceptionbecause it de son hat you That and have a glande ich and beater vields precise detunes to excern right, dans is rander hid and results on estalline Estantino baldings getrand machinder distribution and Arter to constanting it do disfignent behaviour of der Primahle; eis Jogensten, welster dires des primes Assesse, actual Games and Diviceles demalle langere fit good wat hale, and colden hiteraling viele out -ich gonz works and int. thei decrees bestersenting doube onis als Anyeng pernet die me Euler gemache Bemerring, Pon & Produs Euler's product makes the key link JI - - = = = = = = , between Primes and ζ mention polle Prograde, for malle game 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)



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

ALGORITHMIC PROPERTIES

J Borwein

Abacus User and Computer Racer

D Borwein Slide Rule User

P Borwein Grid

(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.



PSLQ and Normality of Digits



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

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

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

Consider the hex digit stream:

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

✓ We have checked 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- π computations from 1986 to 2001

$$y_{1} = \frac{1 - \sqrt[4]{1 - y_{0}^{4}}}{1 + \sqrt[4]{1 - y_{0}^{4}}}, a_{1} = a_{0}(1 + y_{1})^{4} - 2^{3}y_{1}(1 + y_{1} + y_{1}^{2}) \qquad y_{11} = \frac{1 - \sqrt[4]{1 - y_{10}^{4}}}{1 + \sqrt[4]{1 - y_{10}^{4}}}, a_{11} = a_{10}(1 + y_{11})^{4} - 2^{23}y_{11}(1 + y_{11} + y_{11}^{2}) \\ y_{2} = \frac{1 - \sqrt[4]{1 - y_{1}^{4}}}{1 + \sqrt[4]{1 - y_{1}^{4}}}, a_{2} = a_{1}(1 + y_{2})^{4} - 2^{5}y_{2}(1 + y_{2} + y_{2}^{2}) \qquad y_{12} = \frac{1 - \sqrt[4]{1 - y_{11}^{4}}}{1 + \sqrt[4]{1 - y_{11}^{4}}}, a_{12} = a_{11}(1 + y_{12})^{4} - 2^{28}y_{12}(1 + y_{12} + y_{12}^{2}) \\ y_{3} = \frac{1 - \sqrt[4]{1 - y_{2}^{4}}}{1 + \sqrt[4]{1 - y_{2}^{4}}}, a_{3} = a_{2}(1 + y_{3})^{4} - 2^{7}y_{3}(1 + y_{3} + y_{3}^{2}) \qquad y_{13} = \frac{1 - \sqrt[4]{1 - y_{12}^{4}}}{1 + \sqrt[4]{1 - y_{12}^{4}}}, a_{13} = a_{12}(1 + y_{13})^{4} - 2^{27}y_{13}(1 + y_{13} + y_{13}^{2}) \\ y_{4} = \frac{1 - \sqrt[4]{1 - y_{3}^{4}}}{1 + \sqrt[4]{1 - y_{3}^{4}}}, a_{4} = a_{3}(1 + y_{4})^{4} - 2^{9}y_{4}(1 + y_{4} + y_{4}^{2}) \qquad y_{14} = \frac{1 - \sqrt[4]{1 - y_{13}^{4}}}{1 + \sqrt[4]{1 - y_{14}^{4}}}, a_{14} = a_{13}(1 + y_{14})^{4} - 2^{29}y_{14}(1 + y_{14} + y_{14}^{2}) \\ y_{5} = \frac{1 - \sqrt[4]{1 - y_{4}^{4}}}{1 + \sqrt[4]{1 - y_{4}^{4}}}, a_{5} = a_{4}(1 + y_{5})^{4} - 2^{11}y_{5}(1 + y_{5} + y_{5}^{2}) \qquad y_{15} = \frac{1 - \sqrt[4]{1 - y_{14}^{4}}}{1 + \sqrt[4]{1 - y_{14}^{4}}}, a_{15} = a_{14}(1 + y_{15})^{4} - 2^{31}y_{15}(1 + y_{15} + y_{16}^{2}) \\ y_{6} = \frac{1 - \sqrt[4]{1 - y_{4}^{4}}}{1 + \sqrt[4]{1 - y_{4}^{4}}}, a_{7} = a_{6}(1 + y_{7})^{4} - 2^{16}y_{7}(1 + y_{7} + y_{7}^{2}) \qquad y_{17} = \frac{1 - \sqrt[4]{1 - y_{14}^{4}}}{1 + \sqrt[4]{1 - y_{14}^{4}}}, a_{15} = a_{14}(1 + y_{15})^{4} - 2^{31}y_{15}(1 + y_{17} + y_{17}^{2}) \\ y_{8} = \frac{1 - \sqrt[4]{1 - y_{6}^{4}}}{1 + \sqrt[4]{1 - y_{6}^{4}}}, a_{7} = a_{6}(1 + y_{7})^{4} - 2^{16}y_{7}(1 + y_{7} + y_{7}^{2}) \qquad y_{17} = \frac{1 - \sqrt[4]{1 - y_{16}^{4}}}{1 + \sqrt[4]{1 - y_{16}^{4}}}, a_{18} = a_{17}(1 + y_{18})^{4} - 2^{37}y_{18}(1 + y_{18} + y_{18}^{2}) \\ y_{9} = \frac{1 - \sqrt[4]{1 - y_{6}^{4}}}{1 + \sqrt[4]{1 - y_{6}^{4}}}, a_{9} = a_{8}(1 + y_{9})^{4} - 2^{17}y_{9}(1 + y_{9} + y_{9}^{2}) \qquad y_{18} = \frac{1 - \sqrt[4]{1 - y_{16}^{4}}}{1 + \sqrt[4]{1 -$$

Set
$$a_0 = 6 - 4\sqrt{2}$$
 and $y_0 = \sqrt{2} - 1$. Iterate
 $y_{k+1} = \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}}$ and
 $a_{k+1} = a_k(1 + y_{k+1})^4$
 $- 2^{2k+3}y_{k+1}(1 + y_{k+1} + y_{k+1}^2)$.

Then $1/a_k$ converges quartically to π

A random walk on a million digits of Pi

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- 4. Inverse Symbolic Computation.
 - A problem of Knuth, $\pi/8$, Extreme Quadrature
- **5. The Future is Here.**
 - Examples and Issues
- 6. Conclusion.
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 - ✓ Long Range Plan for HPC in Canada





An Inverse and a Color Calculator

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

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





INVERSE SYMBOLIC CALCULATOR

O Simple Lookup and Browser for any number.	
O Smart Lookup for any number.	
O Generalized Expansions for real numbers of at least 16 digits.	
O Integer Relation Algorithms for any number.	
1 ? 😭 =	

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

 $W \exp(W) = x$



W's Riemann surface

Donald Knuth* asked for a closed form evaluation of:

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

- 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

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





We have certain

knowledge without

proof

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.

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

Extreme Quadrature ... 20,000 Digits 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 in seconds and speedup ratios for all processors 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

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)

Outline. What is HIGH PERFORMANCE MATHEMATICS?

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- 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







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

The future I.





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



a. ACENet and HPC@DAL



WestGrid

Dalhousie Distributed Researc

ACEnet completes the Pan Canadian Consortia



avec le

de ha

CLUME

NCV

Enabling Canadian research excellence through high erformance computing



ACENER

Done

© 2005 ACEnet.ca, All Rights Reserved

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

b. Advanced Knowledge Management

Home News

People

Dalhousie Distributed

Projects include • PSL

- FWDM (IMU)
- CiteSeer

Liniversi

Wester

Ontari

ETT	DALHOUSIE
	UNIVERSITY
	Inspiring Minds

Drive

Privacy and Security Lab



(FWDM)

HALIFAX, NOVA SCOTIA | CANADA B3H 4R2 | +1 (902) 494-2093 Computer Science» Privacy and Security Lab » Home

Mission Statement

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

irtual Environment

ationale

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

Diverse partners include

- International Mathematical Union
- CMS
- Symantec and IBM



Search

c. Advanced Networking

Dalhousie Distributed Research Institute and Virtual Environment

Drive



d. Access Grid, AGATE and Apple



Dalhousie Distributed Research Institute and Virtual Environment

First 25 teachers identified



agente 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

Wednesday, December 15, 2004 Try your hand at new math

BUSINESS

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 compa

raphing calculaftware for hand

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

fessor friends d Jonathan Bor athResources Inc. ted to create new a 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. tow the chairman of inc.'s nine-member ors. There are 30

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

lectronic dictionaries nd we're going to be aughing. y decided to "move nd create software for nts. Let's Do Math:

designed for grades 4 sed in late 1998. ing respectably good product," Mr. Fitzger-

> pleased next year under r. Fitzgerald hopes will

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-Th

Rouald Fileperald, president of Mathikesources Inc., holds a hand-held computer capable of a

eventional computers and running the company's mathemat to explain techs

INCORACTIVE

MATH dictionany



on this project in ery little interest were incredibly

Mr. Fil too gi

MathResources Inc.

mitacs

Par Para



Copyright © 2004 MathResources 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

athResources Inc.

Risurface		surface					
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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					
		v-range From: 0 To: 2*Pi					
		Plot Reset					
	1						
		Elle Style Color Axes Projection					
thata (t) range Erers:		theta (t) range From: -15*cos(2*) To: 10*cos(3*t)					
	2"M						
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 >> Pentagonal number Percent Streentage 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.



Let's Do	Math: Tools & Things			1						T.	
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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

opening, I gave one 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 ✓ At the official April feats of the most memorable futuristic films.

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

from atop ain echoes its al as a facility terina research s whose

The future II. IRMACS at SFU

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.

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

easily upgradeable computational, multimedia, internet and remote conferencing (including satellite) technology. High performance distributed computing and dustering technology, designed at SFU, and annex to West Originan other high an and intermentingial maturals with shound approximation and exciting adju-









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









Mathematical Immersive Reality in Vancouver
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

<u>**2**</u>¹⁷ cpu's

2.9/5.7 TF/s 256 GB DDR

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

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✓ Long Range Plan for HPC in Canada







ENGINES OF DISCOVERY: The 21st Century Revolution

The Long Range Plan for High Performance Computing in Canada





The LRP tells a Story

The Story

 Executive Summary
Main Chapters
Technology
Operations
HQP
Budget

> 25 Case Studies many sidebars

One Day ...

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

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

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

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

WEATHER PREDICTION

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







Dalhousie Distributed Research Institute and Virtual Environment



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."

Enigma

• J. Hadamard quoted at length in E. Borel, *Lecons sur la theorie des fonctions*, 1928.