Experimental Computation and Visual Theorems:
Part I: The Computer as Collaborator

Jonathan Borwein FRSC FAAAS FAA FBAS FAMS
(With Aragón, Bailey, P. Borwein, Skerritt, Straub, Tam, Wan, Zudilin, ...)

CARMA

THE UNIVERSITY OF NEWCASTLE AUSTRALIA

Centre for Computer Assisted Research Mathematics and its Applications
The University of Newcastle, Australia

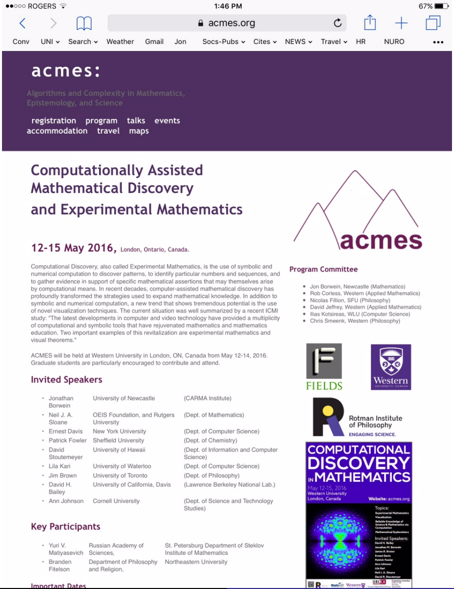
http://carma.newcastle.edu.au/meetings/evims/

http://www.carma.newcastle.edu.au/jon/visuals-ext-abst.pdf

For 2016 Presentations

Revised 13-05-16

Prepared for ACMES, May 12–15, 2016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Algorithms and Complexity in Mathematics, Epistemology, and Science

registration program talks events accommodation travel maps

Computationally Assisted Mathematical Discovery and Experimental Mathematics

12-15 May 2016, London, Ontario, Canada.

Computational Discovery, also called Experimental Mathematics, is the use of symbolic and numerical computation to discover patterns, to identify particular numbers and sequences, and to gather evidence in support of specific mathematical assertions that may themselves arise by computational means. In recent decades, computer-assisted mathematical discovery has profoundly transformed the strategies used to expand mathematical knowledge. In addition to symbolic and numerical computation, a new trend that shows tremendous potential is the use of novel visualization techniques. The current situation was well summarized by a recent ICMI study: "The latest developments in computer and video technology have provided a multiplicity of computational and symbolic tools that have rejuvenated mathematics and mathematics education. Two important examples of this revitalization are experimental mathematics and visual theorems."

ACMES will be held at Western University in London, ON, Canada from May 12-14, 2016. Graduate students are particularly encouraged to contribute and attend.

Invited Speakers

- Jonathan Borwein — University of Newcastle — (CARMA Institute)
- Neil J. A. Sloane — OEIS Foundation, and Rutgers University — (Dept. of Mathematics)
- Ernest Davis — New York University — (Dept. of Computer Science)
- Patrick Fowler — Sheffield University — (Dept. of Chemistry)
- David Stoutemeyer — University of Hawaii — (Dept. of Information and Computer Science)
- Lila Kari — University of Waterloo — (Dept. of Computer Science)
- Jim Brown — University of Toronto — (Dept. of Philosophy)
- David H. Bailey — University of California, Davis — (Lawrence Berkeley National Lab.)
- Ann Johnson — Cornell University — (Dept. of Science and Technology Studies)

Key Participants

- Yuri V. Matiyasevich — Russian Academy of Sciences, — St. Petersburg Department of Steklov Institute of Mathematics
- Branden Fitelson — Department of Philosophy and Religion, — Northeastern University

Important Dates

acmes

Program Committee

- Jon Borwein, Newcastle (Mathematics)
- Rob Corless, Western (Applied Mathematics)
- Nicolas Fillion, SFU (Philosophy)
- David Jeffrey, Western (Applied Mathematics)
- Ilias Kotsireas, WLU (Computer Science)
- Chris Smeenk, Western (Philosophy)

FIELDS

Western

Rotman Institute of Philosophy
ENGAGING SCIENCE.

COMPUTATIONAL DISCOVERY IN MATHEMATICS
May 12-15, 2016
Western University
London, Canada
Website: acmes.org
Topics:
Invited Speakers:

Jacques Hadamard, A Universal Mathematician (1998)

"The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it."–JSH (1865-1963)

last dozen of the first hundred of his year", said at the celebration of Hadamard's centenary:

> The *taupin* who saw Jacques Hadamard enter the lecture theatre, found a teacher who was active, alive, whose reasoning combined exactness and dynamism. Thus the lecture became a struggle and an adventure. Without rigour suffering, the importance of intuition was restored to us, and the better students were delighted. For the others, the intellectual life was less comfortable, but so exciting... And then, above all, we knew quite well that with such a guide we never risked going under [II.5, p. 8].

Mandelbrojt recalled at the same jubilee:

> For several years, Hadamard also gave lectures at the *Collège de France*: lectures which were long, hard, infinitely interesting. He never tried to hide the difficulties, on the contrary he brought them out. The audience thought together with him; these lectures provoked creativity. The day after a lecture by Hadamard was rich, full and all day long one thought about the ideas.
>
> It was in these lectures that I learnt the secrets of the function $\zeta(s)$ of Riemann, it was there that I understood the significance of analytic continuation, of quasi-analyticity, of Dirichlet series, of the role of functional calculus in the calculus of variations [II.5, p. 25-27].

EXTENDED ABSTRACT

Long before current graphic, visualisation and geometric tools were available, John E. Littlewood (1885-1977) wrote in his delightful *Miscellany*[1]:

> *A heavy warning used to be given [by lecturers] that pictures are not rigorous; this has never had its bluff called and has permanently frightened its victims into playing for safety. Some pictures, of course, are not rigorous, but I should say most are (and I use them whenever possible myself). [p. 53]*

[1] J.E. Littlewood, *A mathematician's miscellany*, London: Methuen (1953); Littlewood, J. E. and Bollobás, Béla, ed., *Littlewood's miscellany*, Cambridge University Press, 1986.

Extended Abstract

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Over the past decade, the role of visual computing in my own research has expanded dramatically.

In part this was made possible by the increasing speed and storage capabilities—and the growing ease of programming—of modern multi-core computing environments [BMC].

[1] J.E. Littlewood, *A mathematician's miscellany*, London: Methuen (1953); Littlewood, J. E. and Bollobás, Béla, ed., *Littlewood's miscellany*, Cambridge University Press, 1986.

But, at least as much, it has been driven by my group's paying more active attention to the possibilities for graphing, animating or simulating most mathematical research activities.

[2] See http://www.carma.newcastle.edu.au/jon/Completion.pdf and http://www.carma.newcastle.edu.au/jon/dr-fields11.pptx.

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- *I first briefly discuss both visual theorems and experimental computation.*
- *I then turn to dynamic geometry (iterative reflection methods [AB]) and matrix completion problems (applied to protein conformation [ABT]).*[2] *(Case studies I)*

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- *I then turn to dynamic geometry (iterative reflection methods [AB]) and matrix completion problems (applied to protein conformation [ABT]).*[2] *(Case studies I)*
- *After an algorithmic interlude (Case studies II), I end with description of work from my group in probability (behaviour of short random walks [BS, BSWZ]) and transcendental number theory (normality of real numbers [AB3]). (Case studies III)*

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[2] See `http://www.carma.newcastle.edu.au/jon/Completion.pdf` and `http://www.carma.newcastle.edu.au/jon/dr-fields11.pptx`.

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- What makes most sense for the audience
- My inclinations on the day
- How I manage my time

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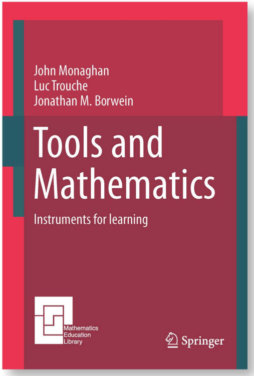
JMB was among roughly 60 new 2015 Fellows of the American Mathematical Society. He was cited "For contributions to nonsmooth analysis and classical analysis as well as experimental mathematics and visualization of mathematics."

Tools and Mathematics April 2016



1st ed. 2016, XXI, 481 p. 133 illus., 92 illus. in color.

Printed book

J. **Monaghan**, L. **Trouche**, J.M. **Borwein**

Tools and Mathematics

Instruments for learning

Series: Mathematics Education Library

- **The only book on the topic of tools and mathematics education**
- **Comprehensive coverage from pre-history to future directions in the field**
- **Content divided equally among the areas of curriculum, assessment, and policy design**

This book is an exploration of tools and mathematics and issues in mathematics education related to tool use. The book has four parts. The first part sets the scene with a reflection on doing a mathematical task with different tools, a mathematician's account of tool use in his work and historical considerations of tool use. The second part opens with a broad review of technology and intellectual trends, circa 1970, and continues with three case studies of approaches in mathematics education and the place of tools in these approaches. The third part considers issues related to mathematics instructions: curriculum, assessment and policy; the calculator debate; mathematics in the real world; and teachers' use of technology. The final part looks to the future and digital tools: task design; the importance of artefacts in gameplay; and new forms of activity via connectivity.

Key References and URLS

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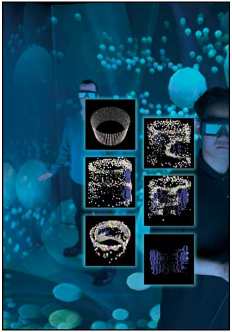
- F. ARAGON, D. H. BAILEY, J.M. BORWEIN AND P.B. BORWEIN, "Walking on real numbers." *Mathematical Intelligencer*. **35**(1) (2013), 42–60.
- F. ARAGON, J. M.BORWEIN, AND M. TAM, '"Douglas-Rachford feasibility methods for matrix completion problems.*ANZIAM Journal*, **55** (4) (2014), 299–326. Available at `http://arxiv.org/abs/1308.4243`.
- J.M. BORWEIN AND A. STRAUB, "Mahler measures, short walks and logsine integrals." *Theoretical Comp Sci*. Special issue on *Symbolic and Numeric Computation*. **479** (1) (2013), 4-21. DOI: `http://link.springer.com/article/10.1016/j.tcs.2012.10.025`.
- J.M. BORWEIN, M. SKERRITT AND C. MAITLAND, "Computation of a lower bound to Giuga's primality conjecture." *Integers* **13** (2013). Online Sept 2013 at #A67, `http://www.westga.edu/~integers/cgi-bin/get.cgi`.
- J.M. BORWEIN, A. STRAUB, J. WAN AND W. ZUDILIN (with an Appendix by Don Zagier), "Densities of short uniform random walks." *Can. J. Math.* **64**(5), (2012), 961-990. `http://dx.doi.org/10.4153/CJM-2011-079-2`.

...and 3D?



NAMS 2005. KnotPlot in a Cave

Considerable obstacles generally present themselves to the beginner, in studying the elements of Solid Geometry, from the practice which has hitherto uniformly prevailed in this country, of never submitting to the eye of the student, the figures on whose properties he is reasoning, but of drawing perspective representations of them upon a plane.

...

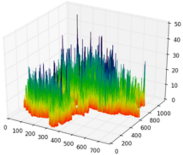
I hope that I shall never be obliged to have recourse to a perspective drawing of any figure whose parts are not in the same plane.—Augustus De Morgan

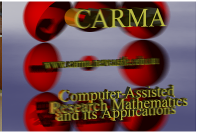
In Adrian Rice,"What Makes a Great Mathematics Teacher?" MAA Monthly, 1999.

Contents

Visual Theorems: Animation, Simulation and Stereo . . .

See `http://vis.carma.newcastle.edu.au/`: Stoneham movie





Cinderella, 3.14 min of Pi, Catalan's constant and Passive 3D

Visual Theorems: Animation, Simulation and Stereo . . .

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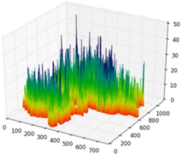
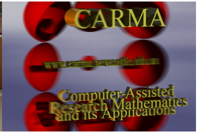
> *The latest developments in computer and video technology have provided a multiplicity of computational and symbolic tools that have rejuvenated mathematics and mathematics education. Two important examples of this revitalization are experimental mathematics* and *visual theorems*
> — *ICMI Study* ***19*** (2012)





Cinderella, 3.14 min of Pi, Catalan's constant and Passive 3D

Contents

Visualising large matrices

Large matrices often have structure that pictures will reveal but which numeric data may obscure.

- The picture shows a 25×25 *Hilbert* matrix on the left and on the right a matrix required to have 50% sparsity and non-zero entries random in $[0, 1]$.

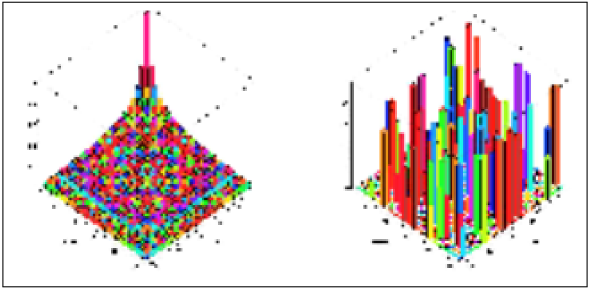


Figure: The Hilbert matrix (L) and a sparse random matrix (R)

Visualising large matrices

MATLAB's first symbolic example

The 4×4 Hilbert matrix is

$$\begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$$

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Hilbert matrices are notoriously unstable numerically. The left of the Figure shows the inverse of the 20×20 Hilbert matrix computed *symbolically exactly*. The middle shows enormous *numerical errors* if one uses 10 digit precision, and the right even if one uses 20 digits.

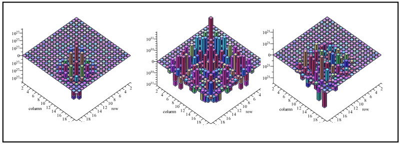

Figure: Inverse 20×20 Hilbert matrix (L) and 2 numerical inverses (R)

Contents

Visualising large polynomials

Large polynomials also often have structure that pictures will reveal but which

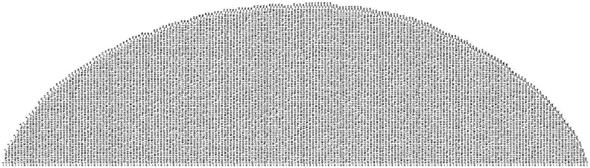

Table: 192-degree minimal polynomial for optical aberration correction, with up to 85 digit coefficients found by multipair PSLQ.

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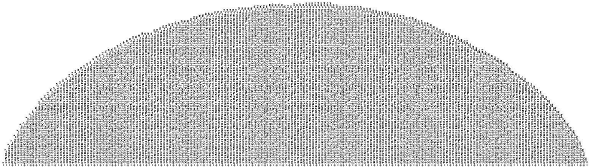

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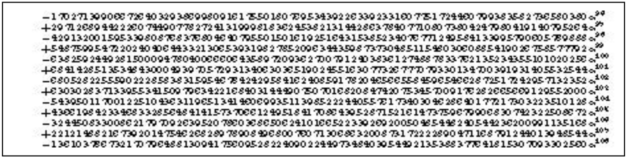


Table: Some large coefficients

Poisson & Crandall for aberration correction

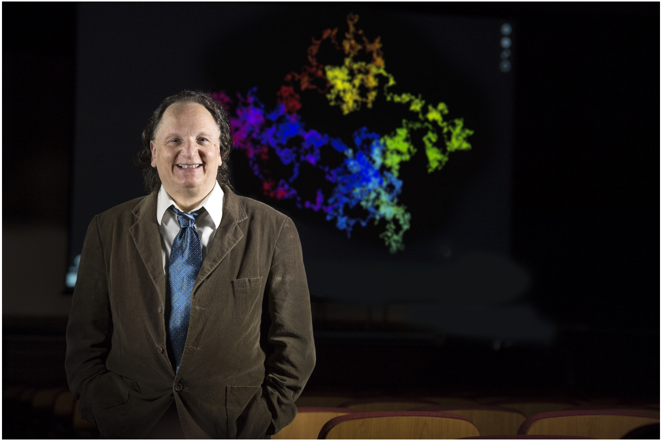
References

- D.H. Bailey, J.M. Borwein, R.E. Crandall and I.J. Zucker, "Lattice sums arising from the Poisson equation." *Journal of Physics A*, **46** (2013) #115201 (31pp).
- D.H. Bailey, J.M. Borwein, and J. Kimberley, "Discovery and computation of large Poisson polynomials." *Experimental Mathematics*, Accepted, May 2016.
- G. Savin and D. Quarfoot, "On attaching coordinates of Gaussian prime torsion points of $y^2 = x^3 + x$ to $Q(i)$," 2010. `www.math.utah.edu/~savin/EllipticCurvesPaper.pdf`[3]

[3] Found from one 12 digit coefficient 387221579866.

Contents

Me and my collaborators



MAA 3.14

http://www.carma.newcastle.edu.au/jon/pi-monthly.pdf

2012 walk on π (went *viral*)

Biggest mathematics picture ever?

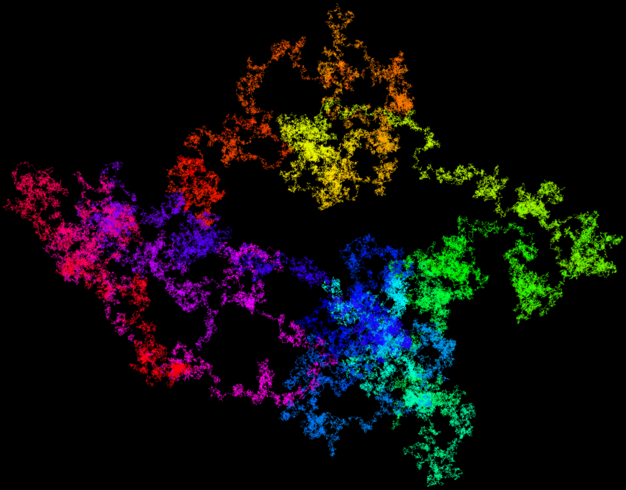


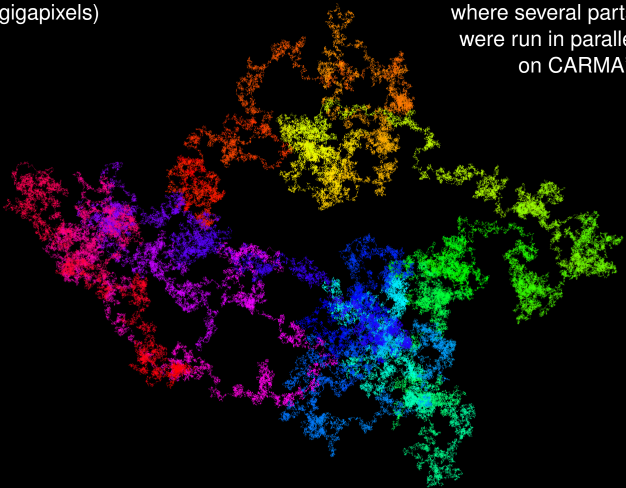
Figure: Walk on first 100 billion base-4 digits of π (normal?).

2012 walk on π (went *viral*)

Biggest mathematics picture ever?

Resolution: $372{,}224 \times 290{,}218$ pixels
(108 gigapixels)

Computation: took roughly a month where several parts of the algorithm were run in parallel with 20 threads on CARMA's MacPro cluster.



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http://gigapan.org/gigapans/106803

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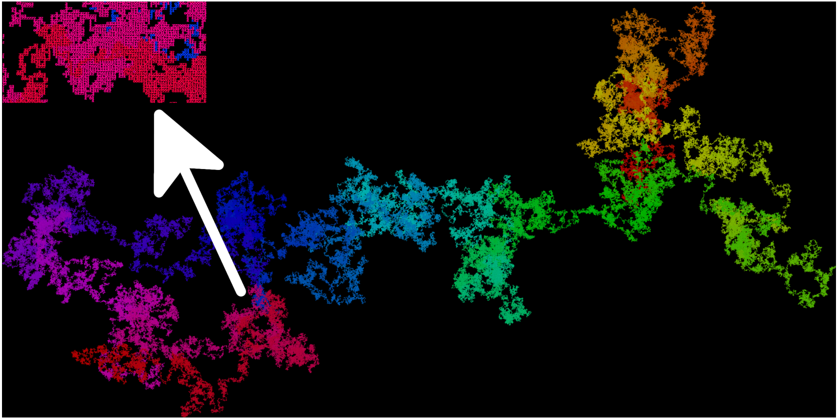


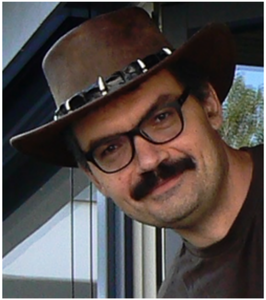
- 100 billion base four digits of π on Gigapan
- Really big pictures are often better than movies (NASA and AMS)

My number-walk collaborators

My short-walk collaborators

James Wan

Armin Straub



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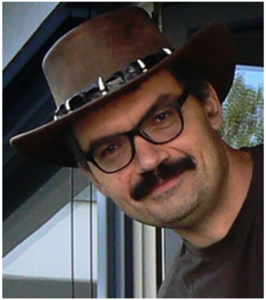

Wadim Zudilin

- Plus Dirk Nuyens  and Don Zagier, ...

Contents

Some early conclusions: So I am sure they get made

Key ideas: randomness, normality of numbers, planar walks, and fractals

How not to experiment

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How not to experiment

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- computations, tables and pictures are experimental data
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- and what you know you can usually use
- you do not need to know much before you start research (as we shall see)

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DHB and JMB, **Exploratory Experimentation in Mathematics** (2011), www.ams.org/notices/201110/rtx111001410p.pdf

Contents

It is not knowledge, but the act of learning, not possession but the act of getting there, which grants the greatest enjoyment.

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When I have clarified and exhausted a subject, then I turn away from it, in order to go into darkness again; the never-satisfied man is so strange if he has completed a structure, then it is not in order to dwell in it peacefully, but in order to begin another.

I imagine the world conqueror must feel thus, who, after one kingdom is scarcely conquered, stretches out his arms for others.

Carl Friedrich Gauss
(1777-1855)

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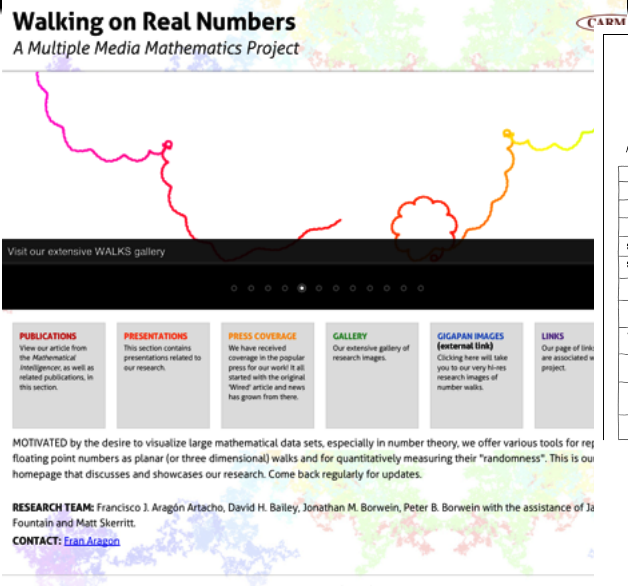
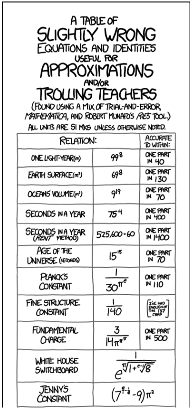
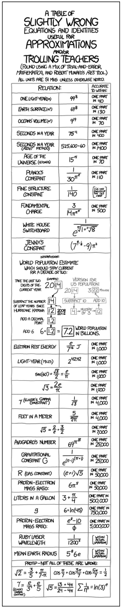
- In an **1808** letter to his friend Farkas (father of Janos) Bolyai
- Archimedes, Euler, Gauss are the big three







Almost all I mention in Part III is accessible at

http://carma.newcastle.edu.au/walks/

Contents

Computer Assisted Research Maths: what it is?

Experimental mathematics is the use of a computer to run computations—sometimes no more than trial-and- error tests—to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search.

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Experimental mathematics is the use of a computer to run computations—sometimes no more than trial-and- error tests—to look for patterns, to identify particular numbers and sequences, to gather evidence in support of specific mathematical assertions that may themselves arise by computational means, including search.

Like contemporary chemists — and before them the alchemists of old—who mix various substances together in a crucible and heat them to a high temperature to see what happens, today's experimental mathematicians put a hopefully potent mix of numbers, formulas, and algorithms into a computer in the hope that something of interest emerges. (JMB-Devlin, *Crucible* 2008, p. 1)

- Quoted in International Council on Mathematical Instruction *Study 19: On Proof and Proving*, 2012

Experimental Mathematics: Integer Relation Methods

Secure Knowledge without Proof. Given real numbers $\beta, \alpha_1, \alpha_2, \ldots, \alpha_n$, Helaman Ferguson's integer relation method (PSLQ), finds a nontrivial linear relation of the form

$$a_0\beta + a_1\alpha_1 + a_2\alpha_2 + \cdots + a_n\alpha_n = 0, \qquad (1)$$

where a_i are integers—if one exists and provides an exclusion bound otherwise.

PROFILE: HELAMAN FERGUSON

Carving His Own Unique Niche, In Symbols and Stone

By refusing to choose between mathematics and art, a self-described "misfit" has found the place where parallel careers meet

CMS D. Borwein Prize: Madelung

2013 Lattice Sums book (CUP)

Experimental Mathematics: Integer Relation Methods

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where a_i are integers—if one exists and provides an exclusion bound otherwise.

- If $a_0 \neq 0$ then (1) assures β is in rational vector space generated by $\{\alpha_1, \alpha_2, \ldots, \alpha_n\}$.

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- **2000** *Computing in Science & Engineering*: PSLQ one of top 10 algorithms of 20th century

(**2001** CISE article on *Grand Challenges* (JB-PB))

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PSLQ in action

In all serious computations of π from 1700 (by John Machin) until 1980 some version of a *Machin formula* was used. These write

$$\arctan(1) = a_1 \cdot \arctan\left(\frac{1}{p_1}\right) + a_2 \cdot \arctan\left(\frac{1}{p_2}\right) + \cdots + a_n \cdot \arctan\left(\frac{1}{p_n}\right) \qquad (2)$$

for rationals $a_1, a_2, \ldots, a_n$ and integers $p_1, p_2, \ldots, p_n > 1$.

Recall the Taylor series $\arctan(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} x^{2n+1}$. Combined with (2) this computes $\pi = 4\arctan(1)$ efficiently, especially if the p_n are not too small.

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For instance, Machin found

$$\pi = 16 \arctan\left(\frac{1}{5}\right) - 4 \arctan\left(\frac{1}{239}\right)$$

while Euler discovered

$$\arctan(1) = \arctan\left(\frac{1}{2}\right) + \arctan\left(\frac{1}{5}\right) + \arctan\left(\frac{1}{8}\right). \tag{3}$$

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- I have a function ‘`pslq`’ in *Maple*. When input data for PSLQ it *predicts* an answer to the precision requested. And checks it to ten digits more (or some other precision).
- This makes the code a real *experimental tool* as it predicts and confirms.

PSLQ in action

prepping for class

```
> pslq(arctan(1),[arctan(1/2),arctan(1/5), arctan(1/8)],20);;
```

[1, 1, 1, 1], "Error is", 0., "checking to", 30, *places*

$$\frac{1}{4}\pi = \arctan\left(\frac{1}{2}\right) + \arctan\left(\frac{1}{5}\right) + \arctan\left(\frac{1}{8}\right)$$

```
> pslq(arctan(1),[arctan(1/2),arctan(1/3), arctan(1/8)],20);
```

[1, 1, 1, 0], "Error is", $-1.\ 10^{-30}$, "checking to", 30, *places*

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```
> pslq(arctan(1),[arctan(1/2),arctan(1/5), arctan(1/9)],20);
```

[42613, 72375, 22013, −40066], "Error is", $2.31604649037\ 10^{-15}$, "checking to", 30, *places*

$$\frac{1}{4}\pi = \frac{72375}{42613}\arctan\left(\frac{1}{2}\right) + \frac{22013}{42613}\arctan\left(\frac{1}{5}\right) - \frac{40066}{42613}\arctan\left(\frac{1}{9}\right)$$

```
> pslq(Pi,[arctan(1/5), arctan(1/239)],20);
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[1, 16, −4], "Error is", $2.8\ 10^{-30}$, "checking to", 30, *places*

$$\pi = 16\arctan\left(\frac{1}{5}\right) - 4\arctan\left(\frac{1}{239}\right)$$

- The third shows that when no relation exists the code may find a good approximation but using very large rationals.

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- The third shows that when no relation exists the code may find a good approximation but using very large rationals.
- So it diagnoses failure because it uses large coefficients and because it is not true to the requested 30 places.

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By digital assistance I mean use of *artefacts* as:

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- Specialized Packages or General Purpose Languages such as Fortran, C++, Python, CPLEX, PARI, SnapPea, and MAGMA.

Digital Assistance

- Web Applications such as: Sloane's Encyclopedia of Integer Sequences, the Inverse Symbolic Calculator, Fractal Explorer, Jeff Weeks' Topological Games, or Euclid in Java.[4]
  - Most of the functionality of the ISC is built into the "identify" function *Maple* starting with version 9.5. For example, `identify(4.45033263602792)` returns $\sqrt{3}+e$. As always, the experienced will extract more than the novice.

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- Web Databases including Google, MathSciNet, ArXiv, GitHub, Wikipedia, MathWorld, MacTutor, Amazon, Wolfram Alpha, the DLMF (all formulas of which are accessible in MathML, as bitmaps, and in TEX) and many more that are not always so viewed.

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All entail *data-mining* . Franklin argues *"exploratory experimentation"* facilitated by *"widening technology"*, as in finance, pharmacology, astrophysics, medicine, and biotechnology, is leading to a reassessment of what legitimates experiment; in that a "*local model*" is not now prerequisite. Sørenson says *experimental mathematics* is following similar tracks.

> *These aspects of exploratory experimentation and wide instrumentation originate from the philosophy of (natural) science and have not been much developed in the context of experimental mathematics. However, I claim that e.g. the importance of wide instrumentation for an exploratory approach to experiments that includes concept formation also pertain to mathematics.*

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In consequence, boundaries between mathematics and natural sciences and between inductive and deductive reasoning are blurred and getting more so.

I leave the philosophically-vexing if mathematically-minor question as to if genuine *mathematical experiments* exist even if one embraces a fully idealist notion of mathematical existence. They sure feel like they do.

Top Ten Algorithms (20C): all but one well used in CARMA

Algorithms for the Ages

"Great algorithms are the poetry of computation," says Francis Sullivan of the Institute for Defense Analyses' Center for Computing Sciences in Bowie, Maryland. He and Jack Dongarra of the University of Tennessee and Oak Ridge National Laboratory have put together a sampling that might have made Robert Frost beam with pride--had the poet been a computer jock. Their list of 10 algorithms having "the greatest influence on the development and practice of science and engineering in the 20th century" appears in the January/February issue of Computing in Science & Engineering. If you use a computer, some of these algorithms are no doubt crunching your data as you read this. The drum roll, please:

1. **1946: The Metropolis Algorithm for Monte Carlo.** Through the use of random processes, this algorithm offers an efficient way to stumble toward answers to problems that are too complicated to solve exactly.
2. **1947: Simplex Method for Linear Programming.** An elegant solution to a common problem in planning and decision-making.
3. **1950: Krylov Subspace Iteration Method.** A technique for rapidly solving the linear equations that abound in scientific computation.
4. **1951: The Decompositional Approach to Matrix Computations.** A suite of techniques for numerical linear algebra.
5. **1957: The Fortran Optimizing Compiler.** Turns high-level code into efficient computer-readable code.
6. **1959: QR Algorithm for Computing Eigenvalues.** Another crucial matrix operation made swift and practical.
7. **1962: Quicksort Algorithms for Sorting.** For the efficient handling of large databases.
8. **1965: Fast Fourier Transform.** Perhaps the most ubiquitous algorithm in use today, it breaks down waveforms (like sound) into periodic components.
9. **1977: Integer Relation Detection.** A fast method for spotting simple equations satisfied by collections of seemingly unrelated numbers.
10. **1987: Fast Multipole Method.** A breakthrough in dealing with the complexity of n-body calculations, applied in problems ranging from celestial mechanics to protein folding.

From *Random Samples*, Science page 799, February 4, 2000.

Experimental Mathematics: PSLQ is core to CARMA

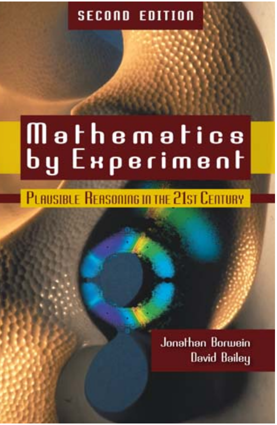
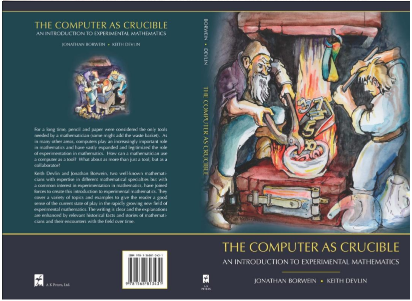
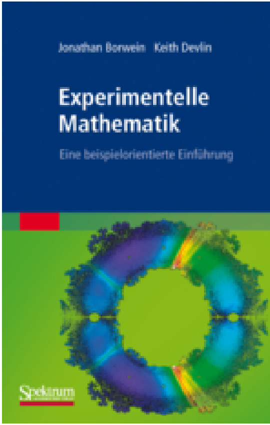


Figure 6.3. Three images quantized at quality 50 (L), 48 (C) and 75 (R). Courtesy of Mason Macklem.





Experimental Mathematics (2004-08, 2009, 2010)

Contents

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Pure mathematicians have not often though of simulation as a relevant tool.
The *cardioid* in the Figure below came from a scatter plot while trying to determine for which complex numbers $z = b/a$ a continued fraction due to Ramanujan, $\mathscr{R}(a,b)$, converged.

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It is given for complex numbers a and b by

$$\mathscr{R}(a,b) = \cfrac{a}{1+\cfrac{b^2}{1+\cfrac{4a^2}{1+\cfrac{9b^2}{1+\ddots}}}}. \tag{4}$$

As often I first tried to compute—$R(1,1)$—and had little luck.

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We eventually determined from highly sophisticated arguments that:

Simulation in pure mathematics

Theorem (Six formulae for $\mathscr{R}(a,a), a>0$)

$$\begin{aligned}
\mathscr{R}(a,a) &= \int_0^\infty \frac{\operatorname{sech}\left(\frac{\pi x}{2a}\right)}{1+x^2}\,\mathrm{d}x \\
&= 2a\sum_{k=1}^\infty \frac{(-1)^{k+1}}{1+(2k-1)a} \\
&= \frac{1}{2}\left(\psi\left(\frac{3}{4}+\frac{1}{4a}\right)-\psi\left(\frac{1}{4}+\frac{1}{4a}\right)\right) \\
&= \frac{2a}{1+a}\,{}_2F_1\left(\left.\begin{matrix}\frac{1}{2a}+\frac{1}{2},1\\ \frac{1}{2a}+\frac{3}{2}\end{matrix}\right|-1\right) \\
&= 2\int_0^1 \frac{t^{1/a}}{1+t^2}\,\mathrm{d}t \\
&= \int_0^\infty e^{-x/a}\operatorname{sech}(x)\,\mathrm{d}x.
\end{aligned}$$

Simulation in pure mathematics

Here ${}_2F_1$ is the hypergeometric function. If you do not know ψ ('psi') , you can easily look it up once you can say 'psi'.
Notice that

$$\mathscr{R}(a,a) = 2\int_0^1 \frac{t^{1/a}}{1+t^2}\,\mathrm{d}t$$

so that $R(1,1) = \log 2$.

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- After making no progress analytically, Crandall and I decided in 2003, taking a somewhat arbitrary criterion for convergence, to colour yellow points for which the fraction seemed to converge.
- We sampled one million points and reasoned a few thousand mis-categorisations would not damage the experiment.

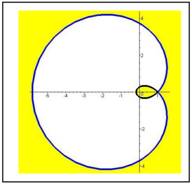

Figure: A cardioid discovered by simulation

Simulation in pure mathematics

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The Figure is so precise that we could identify the cardioid. It is the points where

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Since for positive a, b the fraction satisfies

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

this gave us enormous impetus to continue our eventually successful hunt for a proof.

Contents

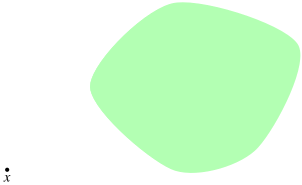
Reflection methods

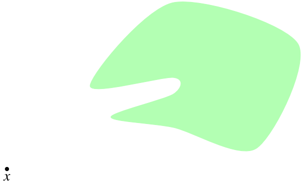
Let $S \subseteq \mathbb{R}^m$. The (nearest point or metric) projection onto S is the (set-valued) mapping,

$$P_S x := \operatorname*{arg\,min}_{s \in S} \|s - x\|.$$

The reflection w.r.t. S is the (set-valued) mapping,

$$R_S := 2P_S - I.$$





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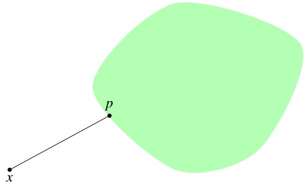

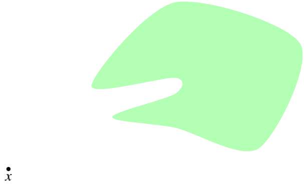

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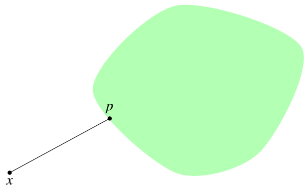

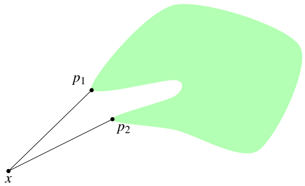

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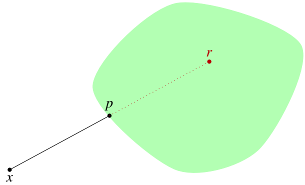

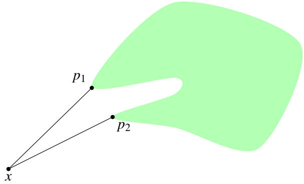

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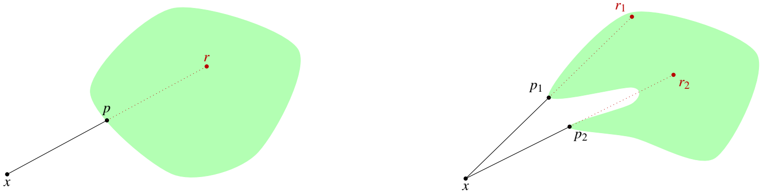
The reflection w.r.t. S is the (set-valued) mapping,

$$R_S := 2P_S - I.$$



The Douglas–Rachford Algorithm (1956–1979–)

Theorem (Douglas–Rachford in finite dimensions)

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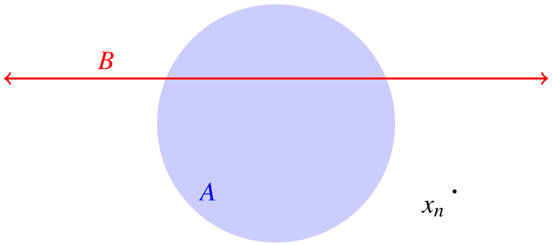

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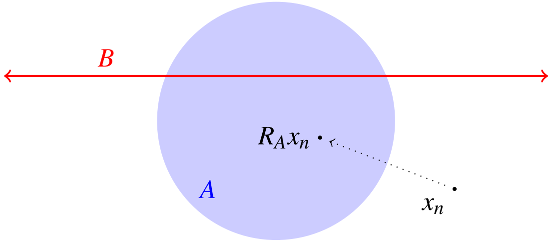

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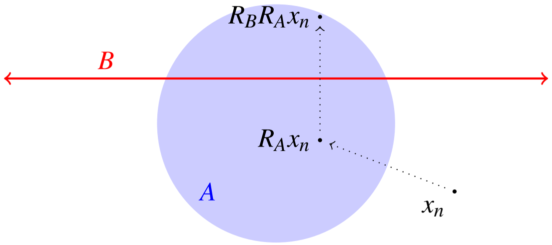

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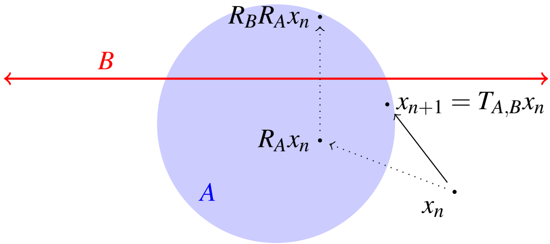

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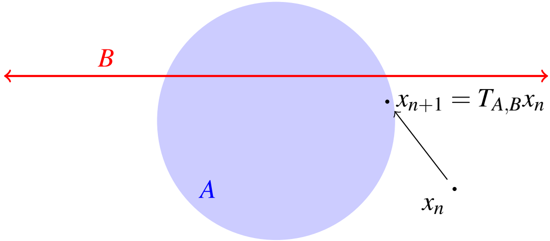

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Works for B affine and A a 'sphere' ANIMATION

In this case we have:

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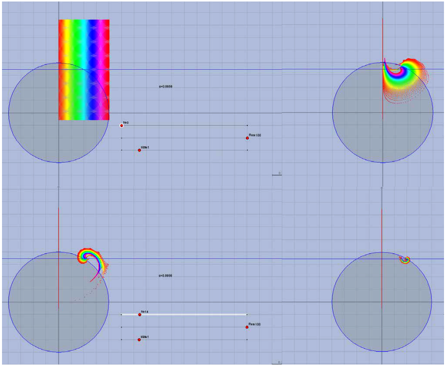
ANIMATION

In this case we have:

- Some local and fewer global convergence results.
- Much empirical evidence for this and other non-convex settings.
  - both numeric and geometric (Cinderella/SAGE)
  - http://carma.newcastle.edu.au/jon/expansion.html



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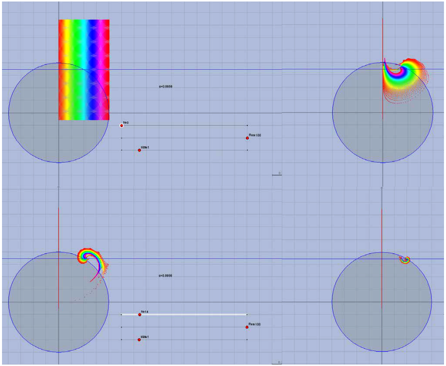

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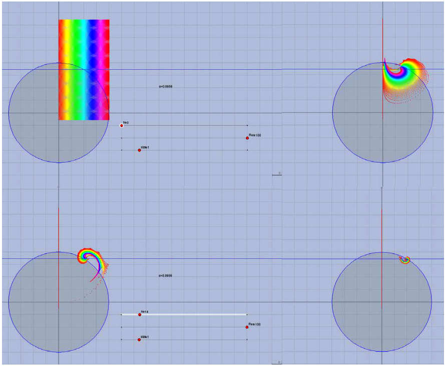

$\Longleftarrow$ **from Cinderella applet**

- 20000 starting points coloured by distance from y-axis
- after $0, 7, 14, 21$ steps
- a "*generic* visual theorem"?

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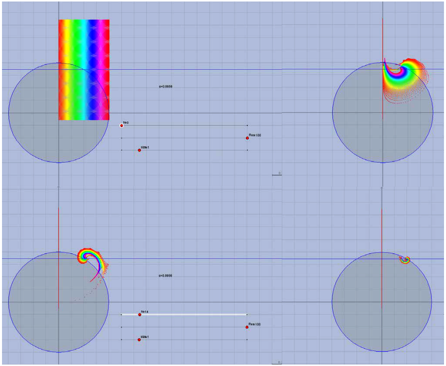

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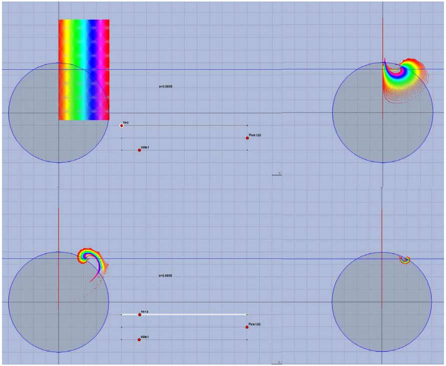

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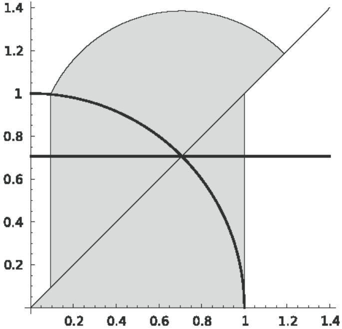
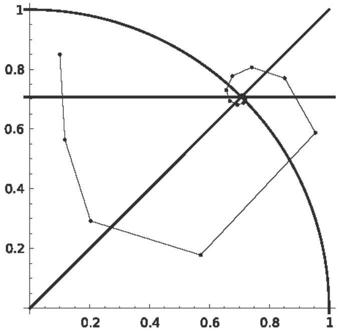
- note the *error* from using only 14 digit computation.

Works for B affine and A a 'sphere'

What we could *prove* (L) and what we could *see* (R)





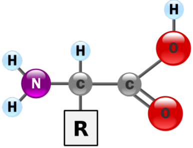
2012 Proven region of convergence in grey

2014 Lyapunov function based proof of global convergence (Benoist)

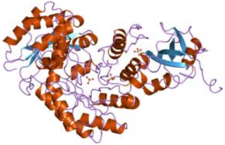
Contents

Case study I: Protein conformation determination

Proteins: large biomolecules comprising multiple amino acid chains.[5]



Generic amino acid



RuBisCO

Matt Tam

[5] RuBisCO (responsible for photosynthesis) has 550 amino acids (smallish).

[6] A coupling which occurs through space, rather than chemical bonds.

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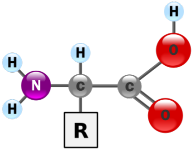

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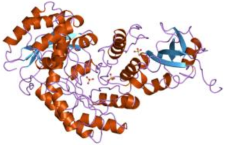

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- Proteins participate in virtually every cellular process !
- Protein structure $\rightarrow$ predicts how functions are performed.
- NMR spectroscopy (Nuclear Overhauser effect[6]) can determine a subset of interatomic distances without damage (under 6Å).

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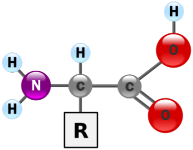

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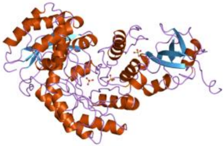

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A *low-rank Euclidean distance matrix completion* problem.

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Six Proteins

Numerics if reconstructed using reflection methods

We use only interatomic distances below 6Å typically constituting less than 8% of the total nonzero entries of the distance matrix.

Table. Six Proteins: average (maximum) errors from five replications.

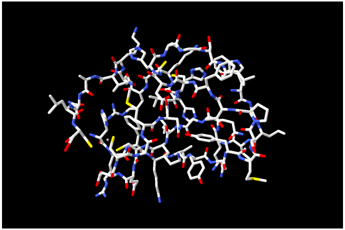
Protein	# Atoms	Rel. Error (dB)	RMSE	Max Error
1PTQ	404	-83.6 (-83.7)	0.0200 (0.0219)	0.0802 (0.0923)
1HOE	581	-72.7 (-69.3)	0.191 (0.257)	2.88 (5.49)
1LFB	641	-47.6 (-45.3)	3.24 (3.53)	21.7 (24.0)
1PHT	988	-60.5 (-58.1)	1.03 (1.18)	12.7 (13.8)
1POA	1067	-49.3 (-48.1)	34.1 (34.3)	81.9 (87.6)
1AX8	1074	-46.7 (-43.5)	9.69 (10.36)	58.6 (62.6)

$$\text{Rel. error}(dB) := 10\log_{10}\left(\frac{\|P_{C_2}P_{C_1}X_N - P_{C_1}X_N\|^2}{\|P_{C_1}X_N\|^2}\right),$$

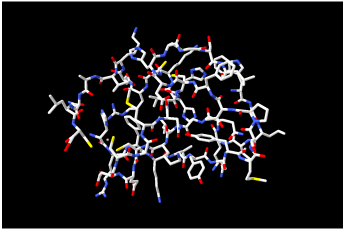
$$\text{RMSE} := \sqrt{\frac{\sum_{i=1}^m \|\hat{p}_i - p_i^{true}\|_2^2}{\text{\# of atoms}}}, \qquad \text{Max} := \max_{1\le i\le m} \|\hat{p}_i - p_i^{true}\|_2.$$

- The points $\hat{p}_1,\hat{p}_2,\ldots,\hat{p}_n$ denote the best fitting of $p_1,p_2,\ldots,p_n$ when rotation, translation and reflection is allowed.

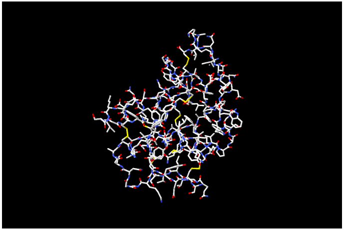
What do the reconstructions look like?



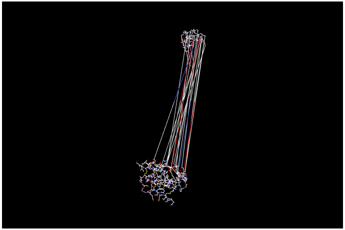
1PTQ (actual)



5,000 steps, -83.6dB (perfect)



1POA (actual)



5,000 steps, -49.3dB (mainly good!)

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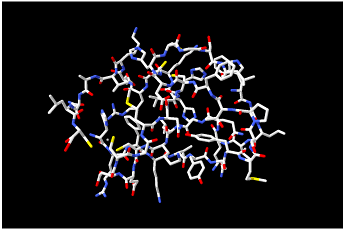

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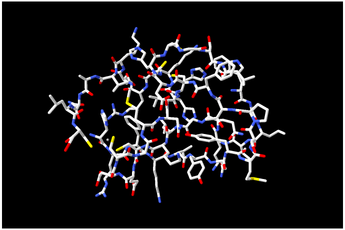

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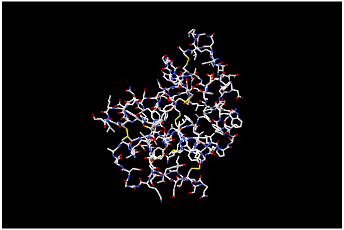

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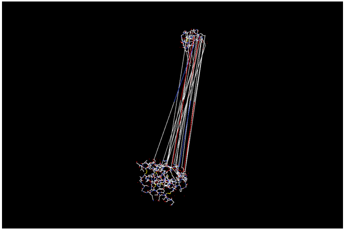

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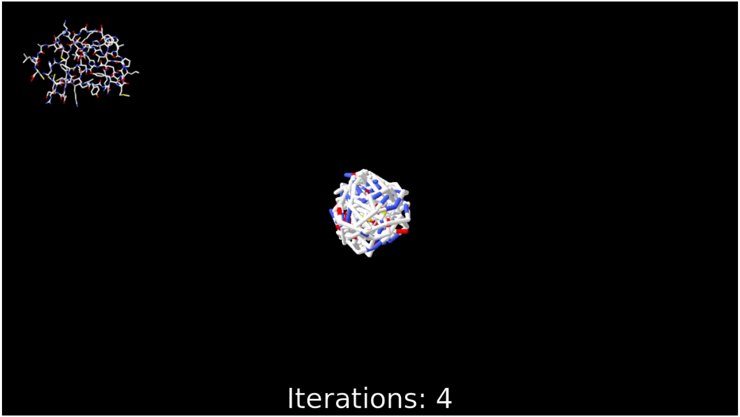
- The picture of 'failure' suggests many strategies

What do reconstructions look like?



Video: First 3,000 steps of the 1PTQ reconstruction.

At `http://carma.newcastle.edu.au/DRmethods/1PTQ.html`

What do the Reconstructions Look Like?

An optimised implementation gave a ten-fold speed-up.

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An optimised implementation gave a ten-fold speed-up. This allowed for the following experiment to be performed:

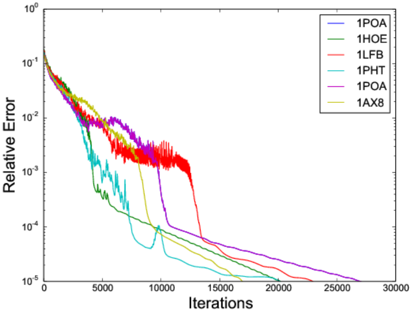

Figure: Relative error by iterations (vertical axis logarithmic).

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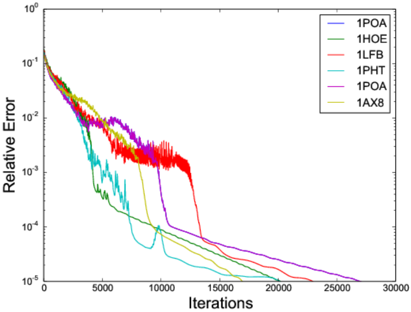
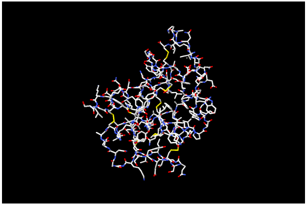


Figure: Relative error by iterations (vertical axis logarithmic).

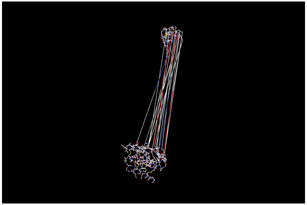
- For $< 5,000$ iterations, the error exhibits non-monotone oscillatory behaviour. It then decreases sharply. Beyond this progress is slower.
- Is early termination to blame? Terminate when error < -100dB.

A More Robust Stopping Criterion

The "un-tuned" implementation (from previous slide):



1POA (actual)



5,000 steps (∼2d), -49.3dB

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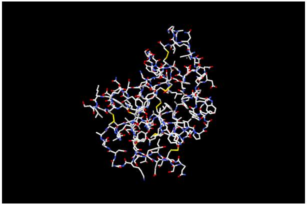

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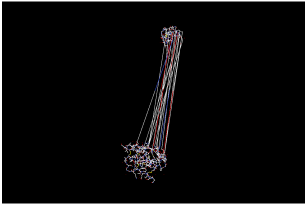

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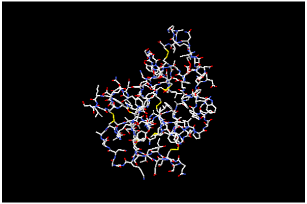

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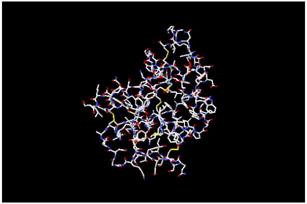

28,500 steps (∼1d), -100dB (perfect!)

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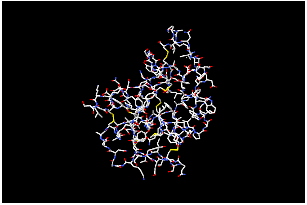

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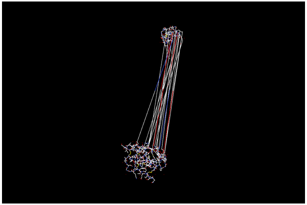

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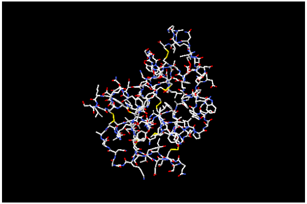

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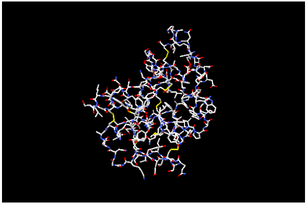


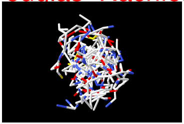
28,500 steps (∼1d), -100dB (perfect!)

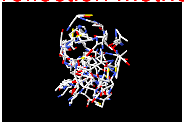
- Similar results observed for the other test proteins.

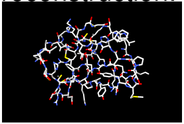
What do reconstructions look like?

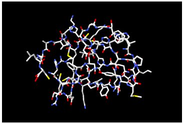
There are many projection methods, so why use Douglas-Rachford?

Douglas–Rachford reflection method reconstruction:

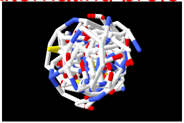

500 steps, -25 dB.

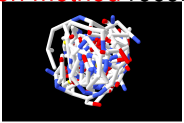

1,000 steps, -30 dB.

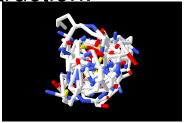

2,000 steps, -51 dB.

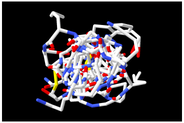

5,000 steps, -84 dB.

Alternating projection method reconstruction:


500 steps, -22 dB.


1,000 steps, -24 dB.

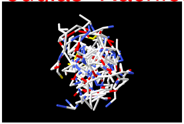

2,000 steps, -25 dB.


5,000 steps, -28 dB.

What do reconstructions look like?

There are many projection methods, so why use Douglas-Rachford?

Douglas–Rachford reflection method reconstruction:



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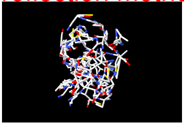
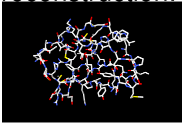
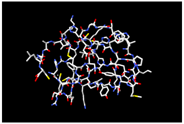


1,000 steps, -30 dB.

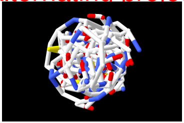


2,000 steps, -51 dB.

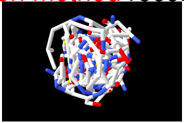


5,000 steps, -84 dB.

Alternating projection method reconstruction:



500 steps, -22 dB.



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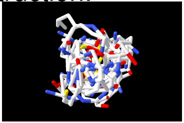

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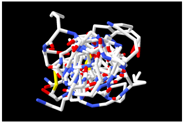

5,000 steps, -28 dB.

- Yet MAP works very well for optical abberation correction (Hubble, amateur telescopes).

Why?

Contents

How the mathematical software world has changed

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> *"If anyone gets 50 digits in total, I will be impressed."*

- To his surprise, a total of **94** teams, representing 25 different nations, submitted results. Twenty of these teams received a full 100 points (10 correct digits for each problem).
- Bailey, Fee and I quit at 85 digits!

The hundred digit challenge

▸ SKIP

The problems and solutions are dissected most entertainingly in

[1] F. Bornemann, D. Laurie, S. Wagon, and J. Waldvogel (2004).“The Siam 100-Digit Challenge: A Study In High-accuracy Numerical Computing”, SIAM, Philadelphia.

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- In a 2005 *Math Intelligencer* review of [1], I wrote

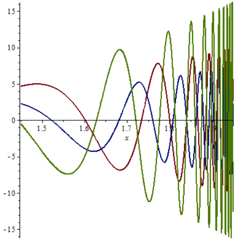
> *Success in solving these problems required a broad knowledge of mathematics and numerical analysis, together with significant computational effort, to obtain solutions and ensure correctness of the results. As described in [1] the strengths and limitations of* Maple, Mathematica, MATLAB *(The 3Ms), and other software tools such as PARI or GAP, were strikingly revealed in these ventures.*
>
> *Almost all of the solvers relied in large part on one or more of these three packages, and while most solvers attempted to confirm their results, there was no explicit requirement for proofs to be provided.*

Trefethen's problem #9

The integral

$$I(\alpha) = \int_0^2 [2+\sin(10\alpha)]x^\alpha \sin\left(\frac{\alpha}{2-x}\right) \mathrm{d}x$$

depends on the parameter α. *What is the value* $\alpha \in [0,5]$ *at which* $I(\alpha)$ *achieves its maximum?*



Integrands for some α

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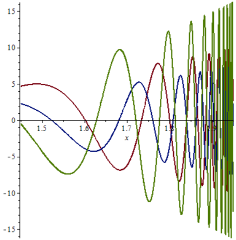


Integrands for some α

- $I(\alpha)$ is expressible in terms of a *Meijer-G function* —a special function with a solid history that we use below.

$$I(\alpha) = 4\sqrt{\pi}\,\Gamma(\alpha)\, G^{3,0}_{2,4}\left(\frac{\alpha^2}{16}\,\middle|\, \begin{matrix}\frac{\alpha+2}{2}, \frac{\alpha+3}{2}\\ \frac{1}{2}, \frac{1}{2}, 1, 0\end{matrix}\right)[\sin(10\,\alpha)+2].$$

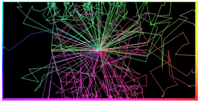
- Unlike most contestants, *Mathematica* and *Maple* will figure this out; help files or a web search then inform the scientist.
- This is another measure of the changing environment. It is usually a good idea—and not at all immoral—to data-mine.

Trefethen's problem #10

ANIMATION

A particle at the center of a 10×1 *rectangle undergoes Brownian motion (i.e., 2-D random walk with infinitesimal step lengths) till it hits the boundary. What is the probability that it hits at one of the ends rather than at one of the sides?*

Walking in a 10×5 box



Trefethen's problem #10 ANIMATION

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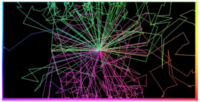
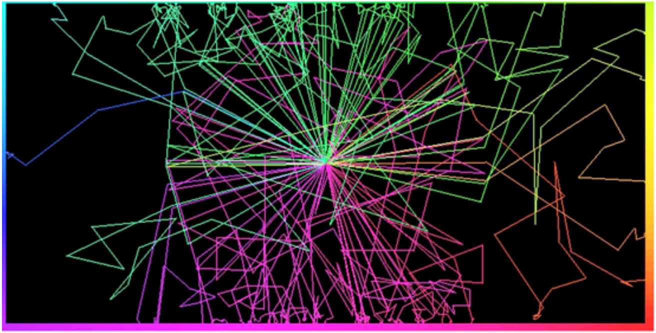


Hitting the Ends. Bornemann [1] starts his remarkable solution by exploring *Monte-Carlo methods*, which are shown to be impracticable.

- He reformulates the problem *deterministically* as *the value at the center of a* 10×1 *rectangle of an appropriate harmonic measure of the ends*, arising from a 5-point discretization of *Laplace's equation* with Dirichlet boundary conditions.
- This is then solved by a well chosen *sparse Cholesky* solver. A reliable numerical value of $3.837587979 \cdot 10^{-7}$ is obtained and the problem is solved *numerically* to the requisite ten places.
- This is the warm up....

Walking in a $b \times a$ box ANIMATION



Trefethen's problem #10

We may proceed to develop two analytic solutions, the *first* using *separation of variables* on the underlying PDE on a general $2a \times 2b$ rectangle. We learn that with $\rho := a/b$

$$p(a,b) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \operatorname{sech}\left(\frac{\pi(2n+1)}{2}\rho\right). \tag{5}$$

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- Three terms yields 50 correct digits:
  $p(10,1) = \underline{0.000000383758797}9251226103407133186204839100793005594 0724\ldots$
- The first term alone, $\frac{4}{\pi}\operatorname{sech}(5\pi)$, gives the underlined digits.

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A *second* method using *conformal mappings*, yields

$$\operatorname{arccot}\rho = p(a,b)\,\frac{\pi}{2} + \arg \mathrm{K}\left(e^{ip(a,b)\pi}\right) \tag{6}$$

where K is the *complete elliptic integral* of the first kind.

Trefethen's problem #10

- We have entered the wonderful world of modular functions

Trefethen's problem #10

- We have entered the wonderful world of modular functions

Bornemann et al ultimately show that the answer is

$$p = \frac{2}{\pi} \arcsin\left(k_{100}\right) \tag{7}$$

where

$$k_{100} := \left(\left(3-2\sqrt{2}\right)\left(2+\sqrt{5}\right)\left(-3+\sqrt{10}\right)\left(-\sqrt{2}+\sqrt[4]{5}\right)^2\right)^2,$$

is a *singular value*. [In general $p(a,b) = \frac{2}{\pi}\arcsin\left(k_{(a/b)^2}\right)$.]

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is a *singular value*. [In general $p(a,b) = \frac{2}{\pi}\arcsin\left(k_{(a/b)^2}\right)$.]

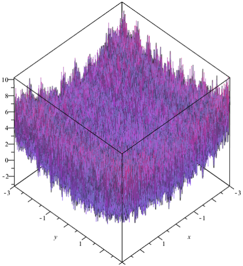
- No one (except harmonic analysts perhaps) anticipated a closed form—let alone one like this.
- Can be done for some other shapes (perhaps, convex with piecewise smooth boundaries, starting at barycentre), and for self-avoiding walks.

Trefethen's problem #4

... zooming

What is the global minimum of the function

$$\exp(\sin(50x)) + \sin(60e^{y}) + \sin(70\sin x) + \sin(\sin(80y)) - \sin(10(x+y)) + (x^2+y^2)/4?$$



Trefethen's problem #4

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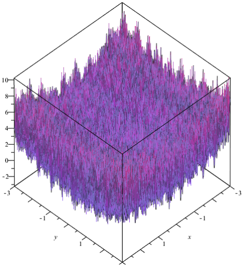
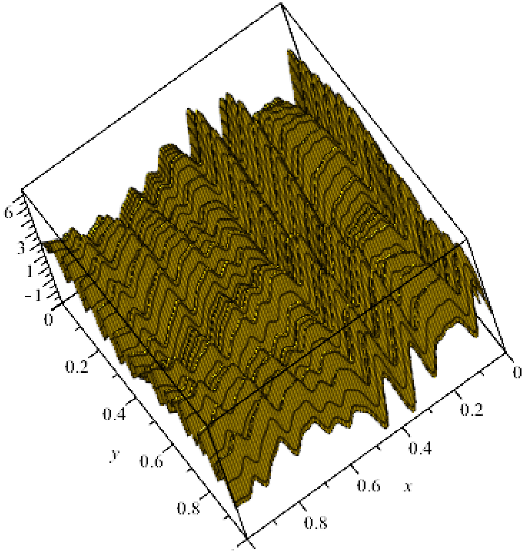


- Can be solved in a global optimization package or by a damped Newton method
- In *Mathematica* by `NMinimize[f[x, y], x, y, Method -> "RandomSearch", "SearchPoints" -> 250, WorkingPrecision -> 20]`
- In *Maple* by `NLPSolve(f(x,y), x = -4 .. 4, y = -4 .. 4, initialpoint = {x = -.4, y = -.1});`
- or by 'zooming' on $[-3,3] \times [-3,3]$.

Trefethen's problem #4

... zooming on [0,1]



Contents

Algorithm performance

a simulated interlude

Proposition (Polylogarithm computation)

(a) For $s = n$ a positive integer,

$$\mathrm{Li}_n(z) = \sum_{m=0}^{\infty}{}' \zeta(n-m) \frac{\log^m z}{m!} + \frac{\log^{n-1} z}{(n-1)!} \left(H_{n-1} - \log(-\log z)\right). \tag{8}$$

(b) For any complex order s not a positive integer,

$$\mathrm{Li}_s(z) = \sum_{m \geq 0} \zeta(s-m) \frac{\log^m z}{m!} + \Gamma(1-s)(-\log z)^{s-1}. \tag{9}$$

Here $\zeta(s) := \sum_n n^{-s}$ and continuations, $H_n := 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n}$, and $\sum'$ avoids the singularity at $\zeta(1)$.

In (8), $|\log z| < 2\pi$ precludes use when $|z| < e^{-2\pi} \approx 0.0018674$. For small $|z|$, however, it suffices to use the definition

$$\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}. \tag{10}$$

Algorithm performance

a simulated interlude

- We found (10) faster than (8) whenever $|z| < 1/4$, for precision from 100 to 4000 digits. We illustrate for Li_2 in the Figure.

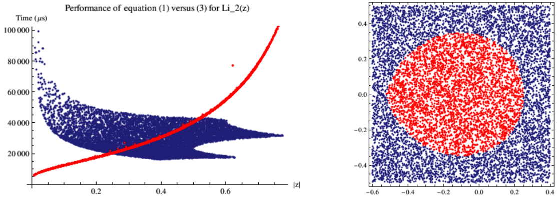
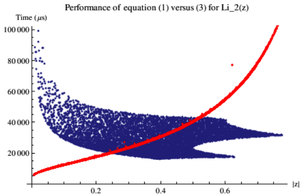


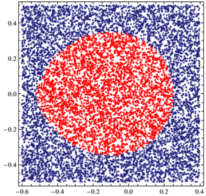
Figure: (L) Timing (8) (blue) and (10) (red).(R) blue region where (8) is faster.

Algorithm performance

a simulated interlude

- We found (10) faster than (8) whenever $|z| < 1/4$, for precision from 100 to 4000 digits. We illustrate for Li_2 in the Figure.
- Timings show microseconds required for $1,000$ digit accuracy as the modulus goes from 0 to 1 with blue showing superior performance of (8). The region records $10,000$ trials of random z, such that $-0.6 < \Re(z) < 0.4, -0.5 < \Im(z) < 0.5$.





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Other References

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