Experimental Mathematics: Examples, Methods and Implications

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The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it. Jacques Hadamard[1]

If mathematics describes an objective world just like physics, there is no reason why inductive methods should not be applied in mathematics just the same as in physics. Kurt Gödel[2]

1 Introduction

Recent years have seen the flowering of "experimental" mathematics, namely the utilization of modern computer technology as an active tool in mathematical research. This development is not limited to a handful of researchers, nor to a handful of universities, nor is it limited to one particular field of mathematics. Instead, it involves hundreds of individuals, at many different institutions, who have turned to the remarkable new computational tools now available to assist in their research, whether it be in number theory, algebra, analysis, geometry or even topology. These tools are being used to work out specific examples, generate plots, perform various algebraic and calculus manipulations, test conjectures, and explore routes to formal proof. Using computer tools to test conjectures is by itself a major time saver for mathematicians, as it permits them to quickly rule out false notions.

Clearly one of the major factors here is the development of robust symbolic mathematics software. Leading the way are the *Maple* and *Mathematica* products, which in the latest

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[1]Quoted at length in E. Borel, *Lecons sur la theorie des fonctions*, 1928.

[2]Kurt Gödel, *Collected Works*, Vol. III, 1951.

editions are far more expansive, robust and user-friendly than when they first appeared 20 to 25 years ago. But numerous other tools, some of which only emerged in the past few years, are also playing key roles. These include: (1) the *Magma* computational algebra package, developed at the University of Sydney in Australia; (2) Neil Sloane's online integer sequence recognition tool, available at `http://www.research.att.com/~njas/sequences`; (3) the inverse symbolic calculator (an online numeric constant recognition facility), available at `http://www.cecm.sfu.ca/projects/ISC`; the electronic geometry site at `http://www.eg-models.de`; and numerous others. See `http://www.experimentalmath.info` for a more complete list, with links to their respective websites.

We must of course also give credit to the computer industry. In 1965, Gordon Moore, before he served as CEO of Intel, observed

> The complexity for minimum component costs has increased at a rate of roughly a factor of two per year. ... Certainly over the short term this rate can be expected to continue, if not to increase. Over the longer term, the rate of increase is a bit more uncertain, although there is no reason to believe it will not remain nearly constant for at least 10 years. [29]

Nearly 40 years later, we observe a record of sustained exponential progress that has no peer in the history of technology. Hardware progress alone has transformed mathematical computations that were once impossible into simple operations that can be done on any laptop.

Many papers have now been published in the experimental mathematics arena, and a full-fledged journal, appropriately titled *Experimental Mathematics*, has been in operation for 12 years. Even older is the AMS journal *Mathematics of Computation*, which has been publishing articles in the general area of computational mathematics since 1960 (since 1943 if you count its predecessor). Just as significant are the hundreds of other recent articles that mention computations, but which otherwise are considered entirely mainstream work. All of this represents a major shift from when the present authors began their research careers, when the view that "real mathematicians don't compute" was widely held in the field.

In this article, we will summarize some of the discoveries and research results of recent years, by ourselves and others, together with a brief description of some of the key methods employed. We will then attempt to ascertain, at a more fundamental level, what these developments mean for the larger world of mathematical research.

2 Integer Relation Detection

One of the key techniques used in experimental mathematics is integer relation detection, which in effect searches for linear relationships satisfied by a set of numerical values. To be precise, given a real or complex vector $(x_1, x_2, \cdots, x_n)$, an integer relation algorithm is a computational scheme that either finds the n integers (a_i), not all zero, such that $a_1x_1 + a_2x_2 + \cdots a_nx_n = 0$ (to within available numerical accuracy), or else establishes that there is no such integer vector within a ball of radius A about the origin, where the metric is the Euclidean norm: $A = (a_1^2 + a_2^2 + \cdots + a_n^2)^{1/2}$. Integer relation computations require very high precision in the input vector x to obtain numerically meaningful results—at least dn-digit precision, where $d = \log_{10} A$. This is the principal reason for the interest in very high-precision arithmetic in experimental mathematics. In one recent integer relation detection computation, 50,000-digit arithmetic was required to obtain the result [9].

At the present time, the best known integer relation algorithm is the PSLQ algorithm [26] of mathematician-sculptor Helaman Ferguson, who, together with his wife Claire, received the 2002 Communications Award of the Joint Policy Board for Mathematics (AMS-MAA-SIAM). Simple formulations of the PSLQ algorithm and several variants are given in [10]. The PSLQ algorithm, together with related lattice reduction schemes such as LLL, was recently named one of ten "algorithms of the century" by the publication *Computing in Science and Engineering* [4]. PSLQ or a variant is implemented in current releases of most computer algebra systems.

3 Arbitrary Digit Calculation Formulas

The best-known application of PSLQ in experimental mathematics is the 1995 discovery, by means of a PSLQ computation, of the "BBP" formula for π:

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

This formula permits one to directly calculate binary or hexadecimal digits beginning at the n-th digit, without needing to calculate any of the first $n-1$ digits [8], using a simple scheme that requires very little memory and no multiple-precision arithmetic software.

It is easiest to see how this individual digit-calculating scheme works by illustrating it for a similar formula, known at least since Euler, for $\log 2$:

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

Note that the binary expansion of $\log 2$ beginning after the first d binary digits is simply $\{2^d \log 2\}$, where by $\{\cdot\}$ we mean fractional part. We can write

$$\begin{aligned} \{2^d \log 2\} &= \left\{ \sum_{n=1}^{\infty} \frac{2^{d-n}}{n} \right\} = \left\{ \sum_{n=1}^{d} \frac{2^{d-n}}{n} \right\} + \left\{ \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \right\} \\ &= \left\{ \sum_{n=1}^{d} \frac{2^{d-n} \bmod n}{n} \right\} + \left\{ \sum_{n=d+1}^{\infty} \frac{2^{d-n}}{n} \right\}, \end{aligned} \tag{2}$$

where we insert "mod n" in the numerator of the first term of (2) since we are only interested in the fractional part after division by n. Now the expression $2^{d-n} \bmod n$ may be evaluated very rapidly by means of the binary algorithm for exponentiation, where each multiplication is reduced modulo n. The entire scheme indicated by formula (2) can be implemented on a computer using ordinary 64-bit or 128-bit arithmetic—high-precision arithmetic software is not required. The resulting floating-point value, when expressed in binary format, gives the first few digits of the binary expansion of $\log 2$ beginning at position $d+1$. Similar calculations applied to each of the four terms in formula (1) yield a similar result for π. The largest computation of this type to date is binary digits of π beginning at the quadrillionth (10^{15}-th) binary digit, performed by an international network of computers organized by Colin Percival.

The BBP formula for π has even found a practical application—it is now employed in the g95 Fortran compiler as part of transcendental function evaluation software.

Since 1995, numerous other formulas of this type have been found and proven, using a similar experimental approach. Several examples include:

$$\pi\sqrt{3} = \frac{9}{32}\sum_{k=0}^{\infty}\frac{1}{64^k}\left(\frac{16}{6k+1}-\frac{8}{6k+2}-\frac{2}{6k+4}-\frac{1}{6k+5}\right) \tag{3}$$

$$\pi^2 = \frac{1}{8}\sum_{k=0}^{\infty}\frac{1}{64^k}\left[\frac{144}{(6k+1)^2}-\frac{216}{(6k+2)^2}-\frac{72}{(6k+3)^2}-\frac{54}{(6k+4)^2}+\frac{9}{(6k+5)^2}\right] \tag{4}$$

$$\begin{aligned}\pi^2 = \frac{2}{27}\sum_{k=0}^{\infty}\frac{1}{729^k}&\left[\frac{243}{(12k+1)^2}-\frac{405}{(12k+2)^2}-\frac{81}{(12k+4)^2}-\frac{27}{(12k+5)^2}\right.\\&\left.-\frac{72}{(12k+6)^2}-\frac{9}{(12k+7)^2}-\frac{9}{(12k+8)^2}-\frac{5}{(12k+10)^2}+\frac{1}{(12k+11)^2}\right]\end{aligned} \tag{5}$$

$$\sqrt{3}\arctan\left(\frac{\sqrt{3}}{7}\right) = \sum_{k=0}^{\infty}\frac{1}{27^k}\left(\frac{3}{3k+1}+\frac{1}{3k+2}\right) \tag{6}$$

$$\frac{25}{2}\log\left[\frac{781}{256}\left(\frac{57-5\sqrt{5}}{57+5\sqrt{5}}\right)^{\sqrt{5}}\right] = \sum_{k=0}^{\infty}\frac{1}{5^{5k}}\left(\frac{5}{5k+2}+\frac{1}{5k+3}\right) \tag{7}$$

Formulas (3) and (4) permit arbitrary-position binary digits to be calculated for $\pi\sqrt{3}$ and π^2. Formulas (5) and (6) permit the same for ternary (base-3) expansions of π^2 and $\sqrt{3}\arctan(\sqrt{3}/7)$. Formula (7) permits the same for the base-5 expansion of the curious constant shown. A compendium of known BBP-type formulas, with references, is available at [5].

One interesting twist here is that the hyperbolic volume of one of Ferguson's sculptures (the "Figure-Eight Knot Complement"[3]—see Figure 1), which is given by

$$V = 2\sqrt{3}\sum_{n=1}^{\infty}\frac{1}{n\binom{2n}{n}}\sum_{k=n}^{2n-1}\frac{1}{k} = 2.029883212819307250042405108549\ldots,$$

has been identified in terms of a BBP-type formula, by application of Ferguson's own PSLQ algorithm. In particular, British physicist David Broadhurst found in 1998, using

[3]Reproduced by permission of the sculptor.

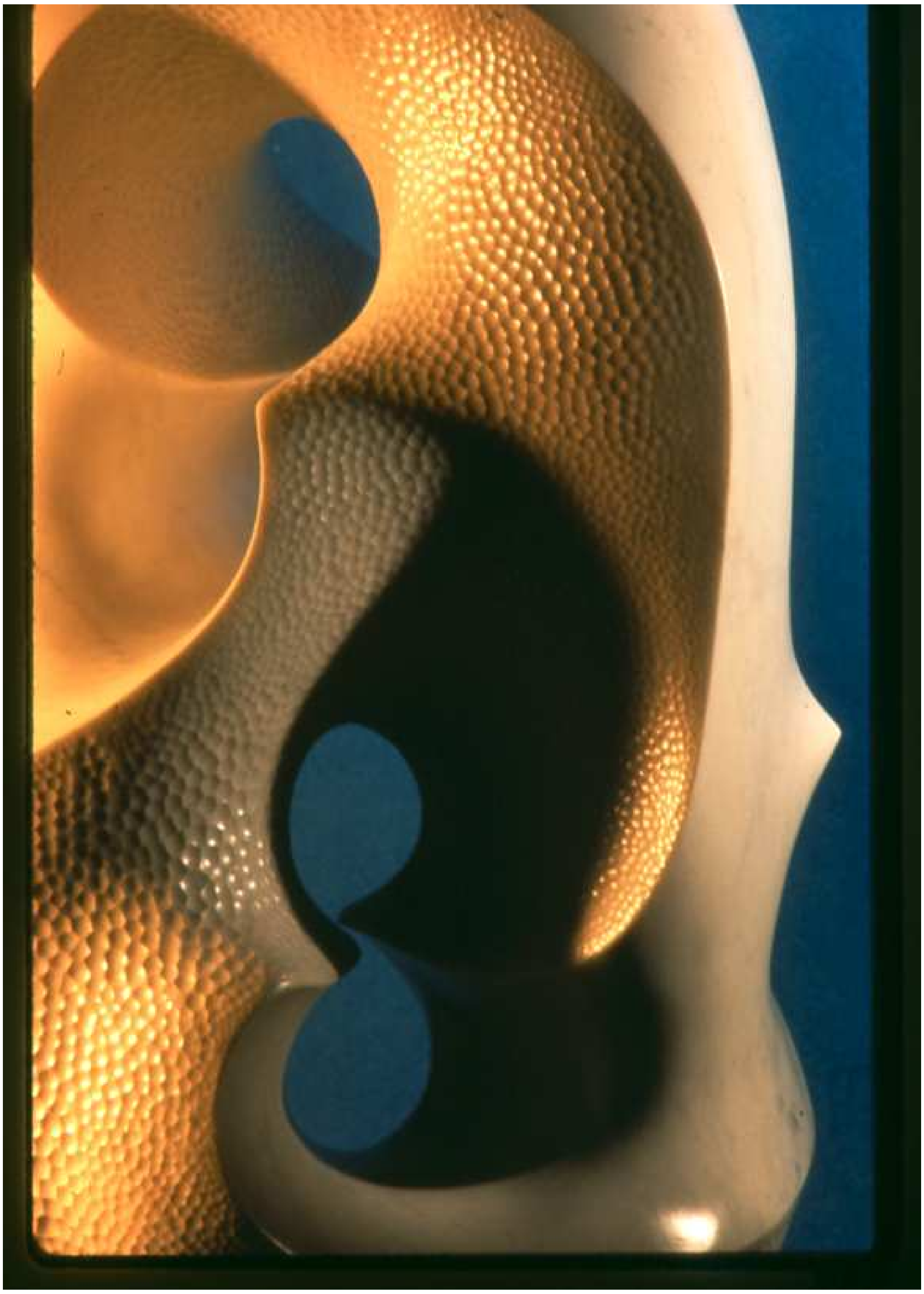

Figure 1: Ferguson's "Figure Eight Knot Complement" sculpture

a PSLQ program, that

$$V = \frac{\sqrt{3}}{9}\sum_{n=0}^{\infty}\frac{(-1)^n}{27^n}\left[\frac{18}{(6n+1)^2}-\frac{18}{(6n+2)^2}-\frac{24}{(6n+3)^2}-\frac{6}{(6n+4)^2}+\frac{2}{(6n+5)^2}\right].$$

This result is proven in [15, Chap. 2, Prob. 34].

4 Does Pi Have a Nonbinary BBP Formula?

Since the discovery of the BBP formula for π in 1995, numerous researchers have investigated, by means of computational searches, whether there is a similar formula for calculating arbitrary digits of π in other number bases (such as base 10). Alas, these searches have not been fruitful.

Recently one of the present authors (JMB), together with David Borwein (Jon's father) and William Galway, established that there is no degree-1 BBP-type formula for π for bases other than powers of two (although this does not rule out some other scheme for calculating individual digits). We will sketch this result here. Full details and some related results can be found in [20].

In the following, $\Re(z)$ and $\Im(z)$ denote the real and imaginary parts of z, respectively. The integer $b > 1$ is not a *proper power* if it cannot be written as c^m for any integers c and $m > 1$. We will use the notation $\mathrm{ord_p(z)}$ to denote the p-adic order of the rational $z \in Q$. In particular, $\mathrm{ord_p(p)} = 1$ for prime p, while $\mathrm{ord_p(q)} = 0$ for primes $q \neq p$, and $\mathrm{ord_p(wz)} = \mathrm{ord_p(w)} + \mathrm{ord_p(z)}$. The notation $\nu_b(p)$ will mean the order of the integer b in the multiplicative group of the integers modulo p. We will say that p is a *primitive prime factor* of $b^m - 1$ if m is the least integer such that $p|(b^m - 1)$. Thus p is a primitive prime factor of $b^m - 1$ provided $\nu_b(p) = m$. Given the Gaussian integer $z \in Q[i]$ and the rational prime $p \equiv 1 \pmod 4$, let $\theta_p(z)$ denote $\mathrm{ord_{\mathfrak{p}}(z)} - \mathrm{ord_{\overline{\mathfrak{p}}}(z)}$, where $\mathfrak{p}$ and $\overline{\mathfrak{p}}$ are the two conjugate Gaussian primes dividing p, and where we require $0 < \Im(\mathfrak{p}) < \Re(\mathfrak{p})$ to make the definition of θ_p unambiguous. Note that

$$\theta_p(wz) = \theta_p(w) + \theta_p(z). \tag{8}$$

Given $\kappa \in R$, with $2 \leq b \in Z$ and b not a proper power, we say that κ has a Z-linear or Q-linear *Machin-type BBP arctangent formula* to the base b if and only if κ can be written as a Z-linear or Q-linear combination (respectively) of generators of the form

$$\arctan\left(\frac{1}{b^m}\right) = \Im\log\left(1+\frac{i}{b^m}\right) = b^m\sum_{k=0}^{\infty}\frac{(-1)^k}{b^{2mk}(2k+1)}. \tag{9}$$

We shall also use the following result, first proved by Bang in 1886:

Theorem 1 *The only cases where $b^m - 1$ has no primitive prime factor(s) are when $b = 2, m = 6, b^m - 1 = 3^2 \cdot 7$ or when $b = 2^N - 1, N \in Z, m = 2, b^m - 1 = 2^{N+1}(2^{N-1} - 1)$.*

We can now state the main result:

Theorem 2 *Given $b > 2$ and not a proper power, then there is no Q-linear Machin-type BBP arctangent formula for π.*

Proof: It follows immediately from the definition of a Q-linear Machin-type BBP arctangent formula that any such formula has the form

$$\pi \;=\; \frac{1}{n}\sum_{m=1}^{M} n_m \Im \log(b^m - i), \tag{10}$$

where $n > 0 \in Z$, $n_m \in Z$, and $M \geq 1$, $n_M \neq 0$. This implies that

$$\prod_{m=1}^{M} (b^m - i)^{n_m} \in e^{ni\pi} Q^{\times} \;=\; Q^{\times}. \tag{11}$$

For any $b > 2$ and not a proper power we have $M_b \leq 2$, so it follows from Bang's Theorem that $b^{4M} - 1$ has a primitive prime factor, say p. Furthermore, p must be odd, since $p = 2$ can only be a *primitive* prime factor of $b^m - 1$ when b is odd and $m = 1$. Since p is a primitive prime factor, it does not divide $b^{2M} - 1$, and so p must divide $b^{2M} + 1 = (b^M + i)(b^M - i)$. We cannot have both $p|b^M + i$ and $p|b^M - i$, since this would give the contradiction that $p|(b^M + i) - (b^M - i) = 2i$. It follows that $p \equiv 1 \pmod 4$, and that p factors as $p = \mathfrak{p}\overline{\mathfrak{p}}$ over $Z[i]$, with exactly one of $\mathfrak{p}$, $\overline{\mathfrak{p}}$ dividing $b^M - i$. Referring to the definition of θ, we see that we must have $\theta_p(b^M - i) \neq 0$. Furthermore, for any $m < M$, neither $\mathfrak{p}$ nor $\overline{\mathfrak{p}}$ can divide $b^m - i$ since this would imply $p \mid b^{4m} - 1$, $4m < 4M$, contradicting the fact that p is a primitive prime factor of $b^{4M} - 1$. So for $m < M$, we have $\theta_p(b^m - i) = 0$. Referring to equation (10), using Equation (8) and the fact that $n_M \neq 0$, we get the contradiction

$$0 \;\neq\; n_M \theta_p(b^M - i) \;=\; \sum_{m=1}^{M} n_m \theta_p(b^m - i) \;=\; \theta_p(Q^{\times}) = 0. \tag{12}$$

Thus our assumption that there was a b-ary Machin-type BBP arctangent formula for π must be false.

5 Normality Implications of the BBP Formulas

One interesting (and unanticipated) discovery is that the existence of these computer-discovered BBP-type formulas has implications for the age-old question of normality for several basic mathematical constants, including π and $\log 2$. What's more, this line of research has recently led to a full-fledged proof of normality for an uncountably infinite class of explicit real numbers.

Given a positive integer b, we will define a real number α to be b-normal if every m-long string of base-b digits appears in the base-b expansion of α with limiting frequency b^{-m}. In spite of the apparently stringent nature of this requirement, it is well known from measure theory that almost all real numbers are b-normal, for all bases b. Nonetheless, there are very few explicit examples of b-normal numbers, other than the likes of *Champernowne's constant* 0.123456789101112131415... In particular, although computations suggest that virtually all of the well-known irrational constants of mathematics (such as $\pi, e, \gamma, \log 2, \sqrt{2}$, etc.) are normal to various number bases, there is not a single proof—not for any of these constants, not for any number base.

Recently one of the present authors (DHB) and Richard Crandall established the following result.

Let $p(x)$ and $q(x)$ be integer-coefficient polynomials, with $\deg p < \deg q$, and $q(x)$ having no zeroes for positive integer arguments. By an *equidistributed* sequence in the unit interval we mean a sequence (x_n) such that for every subinterval (a, b), the fraction $\#[x_n \in (a, b)]/n$ tends to $b - a$ in the limit. The result is as follows:

Theorem 3 *A constant α satisfying the BBP-type formula*

$$\alpha = \sum_{n=1}^{\infty} \frac{p(n)}{b^n q(n)}$$

is b-normal if and only if the associated sequence defined by $x_0 = 0$ and, for $n \geq 1$, $x_n = \{bx_{n-1} + p(n)/q(n)\}$ (where $\{\cdot\}$ denotes fractional part as before), is equidistributed in the unit interval.

For example, $\log 2$ is 2-normal if and only if the simple sequence defined by $x_0 = 0$ and $\{x_n = 2x_{n-1} + 1/n\}$ is equidistributed in the unit interval. For π, the associated sequence is $x_0 = 0$ and

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

Full details of this result are given in [11] [15, Section 3.8].

It is difficult to know at the present time whether this result will lead to a full-fledged proof of normality for, say, π or $\log 2$. However, this approach has yielded a solid normality proof for another class of reals: Given $r \in [0, 1)$, let r_n be the n-th binary digit of r. Then for each r in the unit interval, the constant

$$\alpha_r = \sum_{n=1}^{\infty} \frac{1}{3^n 2^{3^n + r_n}} \tag{13}$$

is 2-normal and transcendental [12]. What's more, it can be shown that whenever $r \neq s$, then $\alpha_r \neq \alpha_s$. Thus (13) defines an uncountably infinite class of distinct 2-normal, transcendental real numbers. A similar conclusion applies when 2 and 3 in (13) are replaced by any pair of relatively prime integers greater than 1.

Here we will sketch a proof of normality for one particular instance of these constants, namely $\alpha_0 = \sum_{n \geq 1} 1/(3^n 2^{3^n})$. Its associated sequence can be seen to be $x_0 = 0$ and $x_n = \{2x_{n-1} + c_n\}$, where $c_n = 1/n$ if n is a power of 3, and zero otherwise. This associated sequence is a very good approximation to the sequence $(\{2^n \alpha_0\})$ of shifted binary fractions of α_0. In fact, $|\{2^n\alpha_0\} - x_n| < 1/(2n)$. The first few terms of the associated sequence are

$$0,\ 0,\ 0, \frac{1}{3}, \frac{2}{3}, \frac{1}{3}, \frac{2}{3}, \frac{1}{3}, \frac{2}{3},$$
$$\frac{4}{9}, \frac{8}{9}, \frac{7}{9}, \frac{5}{9}, \frac{1}{9}, \frac{2}{9}, \frac{4}{9}, \frac{8}{9}, \frac{7}{9}, \frac{5}{9}, \frac{1}{9}, \frac{2}{9}, \frac{4}{9}, \frac{8}{9}, \frac{7}{9}, \frac{5}{9}, \frac{1}{9}, \frac{2}{9},$$
$$\frac{13}{27}, \frac{26}{27}, \frac{25}{27}, \frac{23}{27}, \frac{19}{27}, \frac{11}{27}, \frac{22}{27}, \frac{17}{27}, \frac{7}{27}, \frac{14}{27}, \frac{1}{27}, \frac{2}{27}, \frac{4}{27}, \frac{8}{27}, \frac{16}{27}, \frac{5}{27}, \frac{10}{27}, \frac{20}{27},$$
$$\frac{13}{27}, \frac{26}{27}, \frac{25}{27}, \frac{23}{27}, \frac{19}{27}, \frac{11}{27}, \frac{22}{27}, \frac{17}{27}, \frac{7}{27}, \frac{14}{27}, \frac{1}{27}, \frac{2}{27}, \frac{4}{27}, \frac{8}{27}, \frac{16}{27}, \frac{5}{27}, \frac{10}{27}, \frac{20}{27},$$
$$\frac{13}{27}, \frac{26}{27}, \frac{25}{27}, \frac{23}{27}, \frac{19}{27}, \frac{11}{27}, \frac{22}{27}, \frac{17}{27}, \frac{7}{27}, \frac{14}{27}, \frac{1}{27}, \frac{2}{27}, \frac{4}{27}, \frac{8}{27}, \frac{16}{27}, \frac{5}{27}, \frac{10}{27}, \frac{20}{27},$$

and so forth. The clear pattern is that of triply repeated segments, each of length $2 \cdot 3^m$, where the numerators range over all integers relatively prime to and less than 3^{m+1}.

Note the very even manner in which this sequence fills the unit interval. Given any subinterval (c, d) of the unit interval, it can be seen that this sequence visits this subinterval no more than $3n(d - c) + 3$ times, among the first n elements, provided that $n > 1/(d - c)$. It can then be shown that the sequence $(\{2^j\alpha\})$ visits (c, d) no more than $8n(d - c)$ times, among the first n elements of this sequence, so long as n is at least $1/(d-c)^2$. The 2-normality of α_0 then follows from a result given in [28, pg. 77]. Further details on these results are given in [15, Sec. 4.3], [6], [12].

6 Euler's Multi-Zeta Sums

In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of one of us (JMB) the curious result

$$\sum_{k=1}^{\infty}\left(1+\frac{1}{2}+\cdots+\frac{1}{k}\right)^2 k^{-2} = 4.59987\ldots \approx \frac{17}{4}\zeta(4) = \frac{17\pi^4}{360} \tag{14}$$

where $\zeta(s) = \sum_{n\geq 1} n^{-s}$ is the Riemann zeta function. Au-Yeung had computed the sum in (14) to 500,000 terms, giving an accuracy of five or six decimal digits. Suspecting that his discovery was merely a modest numerical coincidence, Borwein sought to compute the sum to a higher level of precision. Using Fourier analysis and *Parseval's equation*, he wrote

$$\frac{1}{2\pi}\int_0^{\pi}(\pi - t)^2\log^2(2\sin\frac{t}{2})\,dt = \sum_{n=1}^{\infty}\frac{(\sum_{k=1}^{n}\frac{1}{k})^2}{(n+1)^2}. \tag{15}$$

The series on the right of (15) permits one to evaluate (14), while the integral on the left can be computed using the numerical quadrature facility of *Mathematica* or *Maple*. When he did this, he was surprised to find that the conjectured identity (14) holds to more than 30 digits. We should add here that by good fortune, $17/360 = 0.047222\ldots$ has period one and thus can plausibly be recognized from its first six digits, so that Au-Yeung's numerical discovery was not entirely far-fetched.

Borwein was not aware at the time that (14) follows directly from a 1991 result due to De Doelder, and had even arisen in 1952 as a problem in the *American Mathematical Monthly*. What's more, it turns out that Euler considered some related summations. Perhaps it was just as well that Borwein was not aware of these earlier results—and indeed of a large, quite deep and varied literature [21]—because pursuit of this and similar questions had led to a line of research that continues to the present day.

First define the *multi-zeta* constant

$$\zeta(s_1, s_2, \cdots, s_k) \;:=\; \sum_{n_1>n_2>\cdots>n_k>0} \prod_{j=1}^{k} n_j^{-|s_j|} \sigma_j^{-n_j},$$

where the $s_1, s_2, \ldots, s_k$ are non-zero integers, and the $\sigma_j := \mathrm{signum(s_j)}$. Such constants can be considered as generalizations of the Riemann zeta function at integer arguments, in higher dimensions.

The analytic evaluation of such sums has relied on fast methods for computing their numerical values. One scheme, based on *Hölder Convolution*, is discussed in [22] and implemented in *EZFace+*, an online tool available at `http://www.cecm.sfu.ca/projects/ezface+`. We will illustrate its application to one specific case, namely the analytic identification of the sum

$$S_{2,3} \;=\; \sum_{k=1}^{\infty} \left(1 - \frac{1}{2} + \cdots + (-1)^{k+1}\frac{1}{k}\right)^2 (k+1)^{-3}. \tag{16}$$

Expanding the squared term in (16), we have

$$\sum_{\substack{0<i,j<k \\ k>0}} \frac{(-1)^{i+j+1}}{ijk^3} = -2\,\zeta(3,-1,-1) + \zeta(3,2). \tag{17}$$

Evaluating this in *EZFace+* we quickly obtain

$$\begin{aligned} S_{2,3} \;=\; & 0.1561669333811769158810359096879881936857767098403038729575293544 \\ & 97075037440295791455205653709358147578\ldots. \end{aligned}$$

Given this numerical value, PSLQ or some other integer-relation-finding tool can be used to see if this constant satisfies a rational linear relation of certain constants. Our experience with these evaluations has suggested that likely terms would include: $\pi^5, \pi^4\log(2)$, $\pi^3\log^2(2), \pi^2\log^3(2), \pi\log^4(2), \log^5(2), \pi^2\zeta(3), \pi\log(2)\zeta(3), \log^2(2)\zeta(3), \zeta(5), \mathrm{Li}_5(1/2)$. The result is quickly found to be:

$$\begin{aligned} S_{2,3} \;=\; & 4\,\mathrm{Li}_5\left(\frac{1}{2}\right) - \frac{1}{30}\log^5(2) - \frac{17}{32}\zeta(5) - \frac{11}{720}\pi^4\log(2) + \frac{7}{4}\zeta(3)\log^2(2) \\ & + \frac{1}{18}\pi^2\log^3(2) - \frac{1}{8}\pi^2\zeta(3). \end{aligned}$$

This result has been proven in various ways, both analytic and algebraic. Indeed, all evaluations of sums of the form $\zeta(\pm a_1, \pm a_2, \cdots, \pm a_m)$ with *weight* $w := \sum_k a_m$, for $k < 8$, as in (17) are established.

One general result that is reasonably easily obtained is the following, true for all n:

$$\zeta(\{3\}_n) = \zeta(\{2,1\}_n). \tag{18}$$

On the other hand, a general proof of

$$\zeta(\{2,1\}_n) \stackrel{?}{=} 2^{3n}\zeta(\{-2,1\}_n) \tag{19}$$

remains elusive. There has been abundant evidence amassed to support the conjectured identity (19) since it was discovered experimentally in 1996. The first 85 instances of (19) were recently affirmed in calculations by Petr Lisonek to 1000 decimal place accuracy. Lisonek also checked the case $n = 163$, a calculation that required ten hours run time on a 2004-era computer. The only proof known of (18) is a change of variables in a multiple integral representation which sheds no light on (19) (see [21]).

7 Evaluation of Integrals

This same general strategy of obtaining a high-precision numerical value, then attempting, by means of PSLQ or other numeric-constant recognition facilities, to identify the result as an analytic expression, has recently been applied with significant success to the age-old problem of evaluating definite integrals. Obviously *Maple* and *Mathematica* have some rather effective integration facilities, not only for obtaining analytic results directly, but also for obtaining high-precision numeric values. However, these products do have limitations, and their numeric integration facilities are typically limited to 100 digits or so, beyond which they tend to require an unreasonable amount of run time.

Fortunately, some new methods for numerical integration have been developed that appear to be effective for a broad range of one-dimensional integrals, typically producing up to 1000 digit accuracy in just a few seconds (or at most a few minutes) run time on a 2004-era personal computer, and which are also well-suited for parallel processing [13, 14] [16, pg. 312]. These schemes are based on the *Euler-Maclaurin summation* formula [3, pg. 180], which can be stated as follows: Let $m \geq 0$ and $n \geq 1$ be integers, and define $h = (b-a)/n$ and $x_j = a + jh$ for $0 \leq j \leq n$. Further assume that the function $f(x)$ is at least $(2m+2)$-times continuously differentiable on $[a, b]$. Then

$$\begin{aligned}\int_a^b f(x)\,dx &= h\sum_{j=0}^{n} f(x_j) - \frac{h}{2}\left(f(a) + f(b)\right) \\ &\quad - \sum_{i=1}^{m} \frac{h^{2i}B_{2i}}{(2i)!}\left(f^{(2i-1)}(b) - f^{(2i-1)}(a)\right) - E(h)\end{aligned} \tag{20}$$

where B_{2i} denote the Bernoulli numbers, and

$$E(h) = \frac{h^{2m+2}(b-a)B_{2m+2}f^{2m+2}(\xi)}{(2m+2)!}$$

for some $\xi \in (a, b)$. In the circumstance where the function $f(x)$ and all of its derivatives are zero at the endpoints a and b (as in a smooth, bell-shaped function), the second and third terms of the Euler-Maclaurin formula (20) are zero, and we conclude that the error $E(h)$ goes to zero more rapidly than any power of h.

This principle is utilized by transforming the integral of some C^∞ function $f(x)$ on the interval $[-1, 1]$ to an integral on $(-\infty, \infty)$ using the change of variable $x = g(t)$. Here $g(x)$ is some monotonic, infinitely differentiable function with the property that $g(x) \to 1$ as $x \to \infty$ and $g(x) \to -1$ as $x \to -\infty$, and also with the property that $g'(x)$ and all higher derivatives rapidly approach zero for large positive and negative arguments. In this case we can write, for $h > 0$,

$$\int_{-1}^{1} f(x)\, dx \;=\; \int_{-\infty}^{\infty} f(g(t))g'(t)\, dt \;=\; h \sum_{j=-\infty}^{\infty} w_j f(x_j) + E(h)$$

where $x_j = g(hj)$ and $w_j = g'(hj)$ are abscissas and weights that can be pre-computed. If $g'(t)$ and its derivatives tend to zero sufficiently rapidly for large t, positive and negative, then even in cases where $f(x)$ has a vertical derivative or an integrable singularity at one or both endpoints, the resulting integrand $f(g(t))g'(t)$ is, in many cases, a smooth bell-shaped function for which the Euler-Maclaurin formula applies. In these cases, the error $E(h)$ in this approximation decreases faster than any power of h.

Three suitable g functions are $g_1(t) = \tanh t$, $g_2(t) = \operatorname{erf} t$, and $g_3(t) = \tanh(\pi/2 \cdot \sinh t)$. Among these three, $g_3(t)$ appears to be the most effective for typical experimental math applications. For many integrals, *"tanh-sinh" quadrature*, as the resulting scheme is known, achieves quadratic convergence: reducing the interval h in half roughly doubles the number of correct digits in the quadrature result. This is another case where we have more heuristic than proven knowledge.

As one example, recently the present authors, together with Greg Fee of Simon Fraser University in Canada, were inspired by a recent problem in the *American Mathematical Monthly* [2]. They found by using a tanh-sinh quadrature program, together with a PSLQ integer relation detection program, that if $C(a)$ is defined by

$$C(a) \;=\; \int_0^1 \frac{\arctan(\sqrt{x^2 + a^2})\, dx}{\sqrt{x^2 + a^2}(x^2 + 1)},$$

then

$$C(0) = \pi \log 2/8 + G/2, \quad C(1) \;=\; \pi/4 - \pi\sqrt{2}/2 + 3\arctan(\sqrt{2})/\sqrt{2}$$
$$C(\sqrt{2}) \;=\; 5\pi^2/96.$$

Here $G = \sum_{k \ge 0} (-1)^k/(2k + 1)^2$ is *Catalan's constant*—the simplest number whose irrationality is not established but for which abundant numerical evidence exists. These experimental results then led to the following general result, rigorously established, among others:

$$\int_0^\infty \frac{\arctan(\sqrt{x^2 + a^2})\, dx}{\sqrt{x^2 + a^2}(x^2 + 1)} \;=\; \frac{\pi}{2\sqrt{a^2 - 1}} \left[2\arctan(\sqrt{a^2 - 1}) - \arctan(\sqrt{a^4 - 1})\right].$$

As a second example, recently the present authors empirically determined that

$$\begin{aligned}\frac{2}{\sqrt{3}}\int_0^1 \frac{\log^6(x)\arctan[x\sqrt{3}/(x-2)]}{x+1}\,dx &= \frac{1}{81648}\left[-229635L_3(8)\right.\\
&\quad +29852550L_3(7)\log 3 - 1632960L_3(6)\pi^2 + 27760320L_3(5)\zeta(3)\\
&\quad -275184L_3(4)\pi^4 + 36288000L_3(3)\zeta(5) - 30008L_3(2)\pi^6\\
&\quad \left.-57030120L_3(1)\zeta(7)\right],\end{aligned}$$

where $L_3(s) = \sum_{n=1}^{\infty}[1/(3n-2)^s - 1/(3n-1)^s]$. Based on these experimental results, general results of this type have been conjectured but not yet rigorously established.

A third example is the following:

$$\frac{24}{7\sqrt{7}}\int_{\pi/3}^{\pi/2} \log\left|\frac{\tan t+\sqrt{7}}{\tan t-\sqrt{7}}\right| dt \stackrel{?}{=} L_{-7}(2) \tag{21}$$

where

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

The "identity" (21) has been verified to over 2000 decimal digit accuracy, but a proof is not yet known. It arises from the volume of an ideal tetrahedron in hyperbolic space, [15, pp. 90–91]. For algebraic topology reasons, it is known that the ratio of the left hand to the right hand side of (21) is rational.

A related experimental result, verified to 1000 digit accuracy, is

$$\begin{aligned}0 &\stackrel{?}{=} -2J_2 - 2J_3 - 2J_4 + 2J_{10} + 2J_{11} + 3J_{12} + 3J_{13} + J_{14} - J_{15}\\
&\quad -J_{16} - J_{17} - J_{18} - J_{19} + J_{20} + J_{21} - J_{22} - J_{23} + 2J_{25}\end{aligned}$$

where J_n is the integral in (21), with limits $n\pi/60$ and $(n+1)\pi/60$.

The above examples are ordinary one-dimensional integrals. Two-dimensional integrals are also of interest. Along this line we present a more recreational example discovered experimentally by James Klein—and confirmed by *Monte Carlo* simulation. It is that the expected distance between two random points on different sides of a unit square is

$$\begin{aligned}&\frac{2}{3}\int_0^1\int_0^1 \sqrt{x^2+y^2}\,dx\,dy + \frac{1}{3}\int_0^1\int_0^1 \sqrt{1+(u-v)^2}\,du\,dv\\
&\qquad = \frac{1}{9}\sqrt{2} + \frac{5}{9}\log(\sqrt{2}+1) + \frac{2}{9},\end{aligned}$$

and the expected distance between two random points on different sides of a unit cube is

$$\begin{aligned}&\frac{4}{5}\int_0^1\int_0^1\int_0^1\int_0^1 \sqrt{x^2+y^2+(z-w)^2}\,dw\,dx\,dy\,dz\\
&\qquad +\frac{1}{5}\int_0^1\int_0^1\int_0^1\int_0^1 \sqrt{1+(y-u)^2+(z-w)^2}\,du\,dw\,dy\,dz\\
&\qquad = \frac{4}{75} + \frac{17}{75}\sqrt{2} - \frac{2}{25}\sqrt{3} - \frac{7}{75}\pi + \frac{7}{25}\log\left(1+\sqrt{2}\right) + \frac{7}{25}\log\left(7+4\sqrt{3}\right).\end{aligned}$$

See [7] for details and some additional examples. It is not known whether similar closed forms exist for higher-dimensional cubes.

8 Ramanujan's AGM Continued Fraction

Given $a, b, \eta > 0$, define

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

This continued fraction arises in Ramanujan's *Notebooks*. He discovered the beautiful fact that

$$\frac{R_\eta(a,b) + R_\eta(b,a)}{2} = R_\eta\left(\frac{a+b}{2}, \sqrt{ab}\right).$$

The authors wished to record this in [15], and wished to computationally check the identity. A first attempt to numerically compute $R_1(1,1)$ directly failed miserably, and with some effort only three reliable digits were obtained: $0.693\cdots$. With hindsight, the slowest convergence of the fraction occurs in the mathematically simplest case, namely when $a = b$. Indeed $R_1(1,1) = \log 2$ as the first primitive numerics had tantalizingly suggested.

Attempting a direct computation of $R_1(2,2)$ using a depth of 20000 gives us two digits. Thus we must seek more sophisticated methods. From formula (1.11.70) of [16] we see that for $0 < b < a$,

$$\mathcal{R}_1(a,b) = \frac{\pi}{2} \sum_{n \in \mathrm{Z}} \frac{aK(k)}{K^2(k) + a^2 n^2 \pi^2} \operatorname{sech}\left(n\pi \frac{K(k')}{K(k)}\right), \tag{22}$$

where $k = b/a = \theta_2^2/\theta_3^2, k' = \sqrt{1-k^2}$. Here θ_2, θ_3 are Jacobian theta functions and K is a complete elliptic integral of the first kind.

Writing the previous equation as a Riemann sum, we have

$$\mathcal{R}(a) := \mathcal{R}_1(a,a) = \int_0^\infty \frac{\operatorname{sech}(\pi x/(2a))}{1+x^2} dx = 2a \sum_{k=1}^\infty \frac{(-1)^{k+1}}{1+(2k-1)a}, \tag{23}$$

where the final equality follows from the Cauchy-Lindelof Theorem. This sum may also be written as $\mathcal{R}(a) = \frac{2a}{1+a} F\left(\frac{1}{2a} + \frac{1}{2}, 1; \frac{1}{2a} + \frac{3}{2}; -1\right)$. The latter form can be used in *Maple* or *Mathematica* to determine

$$\mathcal{R}(2) = 0.97499098879872209671990033452 9 \ldots.$$

This constant, as written, is a bit difficult to recognize, but if one first divides by $\sqrt{2}$, one can obtain, using the *Inverse Symbolic Calculator*, an online tool available at the URL `http://www.cecm.sfu.ca/projects/ISC/ISCmain.html`, that the quotient is $\pi/2 - \log(1+\sqrt{2})$. Thus we conclude, experimentally, that

$$\mathcal{R}(2) \quad = \quad \sqrt{2}[\pi/2 - \log(1+\sqrt{2})].$$

Indeed, it follows, see [19], that

$$\mathcal{R}(a) \quad = \quad 2\int_0^1 \frac{t^{1/a}}{1+t^2}\,dt.$$

Note that $\mathcal{R}(1) = \log 2$. No non-trivial closed form is known for $\mathcal{R}(a,b)$ with $a \neq b$, although

$$\mathcal{R}_1\left(\frac{1}{4\pi}\beta\left(\frac{1}{4},\frac{1}{4}\right),\frac{\sqrt{2}}{8\pi}\beta\left(\frac{1}{4},\frac{1}{4}\right)\right) \quad = \quad \frac{1}{2}\sum_{n\in\mathbf{Z}}\frac{\operatorname{sech}(n\pi)}{1+n^2},$$

is close to closed. Here β denotes the classical *Beta function.* It would be pleasant to find a direct proof of (23). Further details are to be found in [19, 17, 16].

Study of these Ramanujan continued fractions has been facilitated by examining the closely related dynamical system $t_0 = 1, t_1 = 1$ and

$$t_n := t_n(a,b) \quad = \quad \frac{1}{n} + \omega_{n-1}\left(1-\frac{1}{n}\right)t_{n-2} \tag{24}$$

where $\omega_n = a^2$ or b^2 (from the Ramanujan continued fraction definition), depending on whether n is even or odd.

If one studies this only based on numerical values, nothing is evident—one only sees that $t_n \to 0$ fairly slowly. However, if we look at this iteration pictorially, we learn significantly more. In particular, if we plot these iterates in the complex plane, and then scale by $\sqrt{n}$, and color the iterations blue or red depending on odd or even n, then some remarkable fine structure appears—see Figure 2. With assistance of such plots, the behavior of these iterates (and the Ramanujan continued fractions) are now quite well understood. These studies have ventured into matrix theory, real analysis and even the theory of martingales from probability theory [19, 17, 18, 23].

There are some exceptional cases. *Jacobsen-Masson theory* [17, 18] shows that the even/odd fractions for $\mathcal{R}_1(i,i)$ behave "chaotically," neither converge. Indeed, when $a = b = i$, $(t_n(i,i))$ exhibit a fourfold quasi-oscillation, as n runs through values mod 4. Plotted versus n, the (real) sequence $t_n(\mathbf{i})$ exhibits the serpentine oscillation of four separate "necklaces." The detailed asymptotic is

$$t_n(i,i) = \sqrt{\frac{2}{\pi}\cosh\frac{\pi}{2}}\,\frac{1}{\sqrt{n}}\left(1+O\left(\frac{1}{n}\right)\right)\times\begin{cases}(-1)^{n/2}\cos(\theta-\log(2n)/2) & n \text{ is even}\\ (-1)^{(n+1)/2}\sin(\theta-\log(2n)/2) & n \text{ odd}\end{cases}$$

where $\theta := \arg\Gamma((1+i)/2)$.

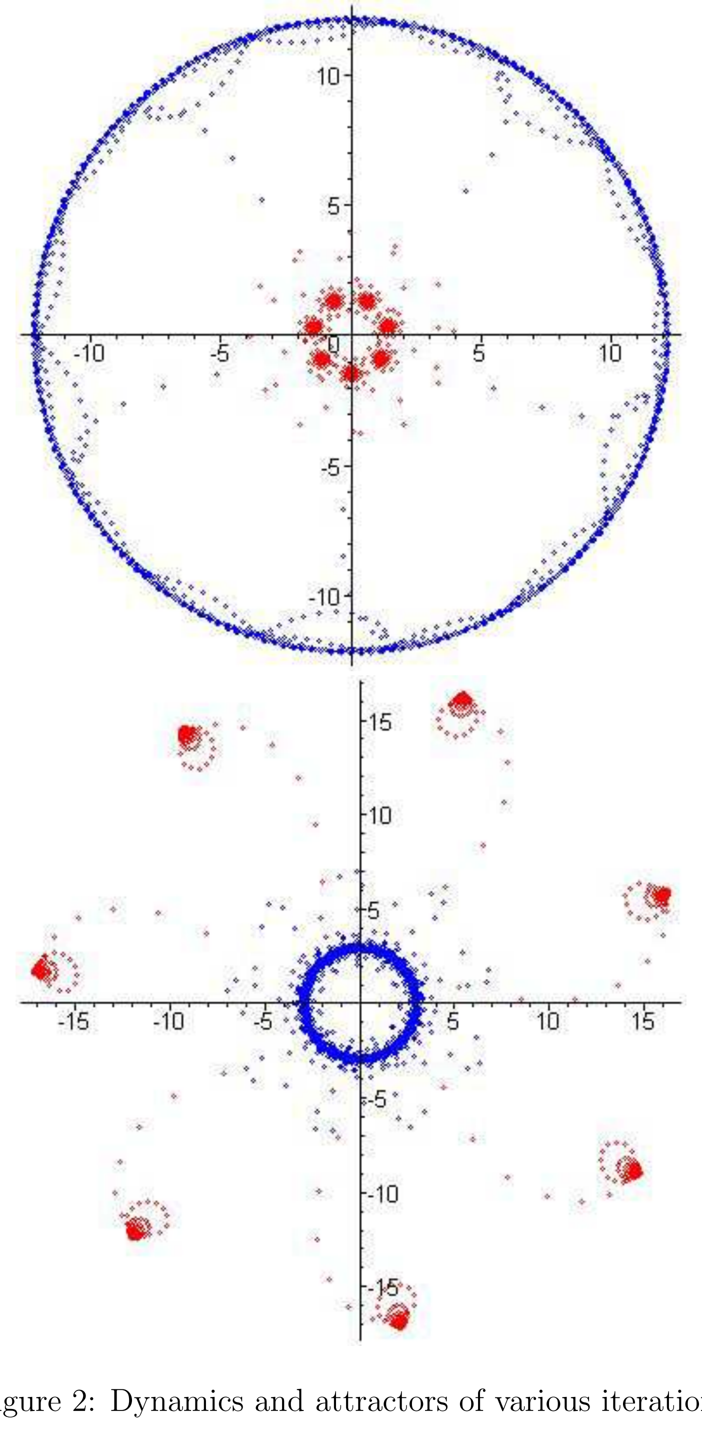

Figure 2: Dynamics and attractors of various iterations

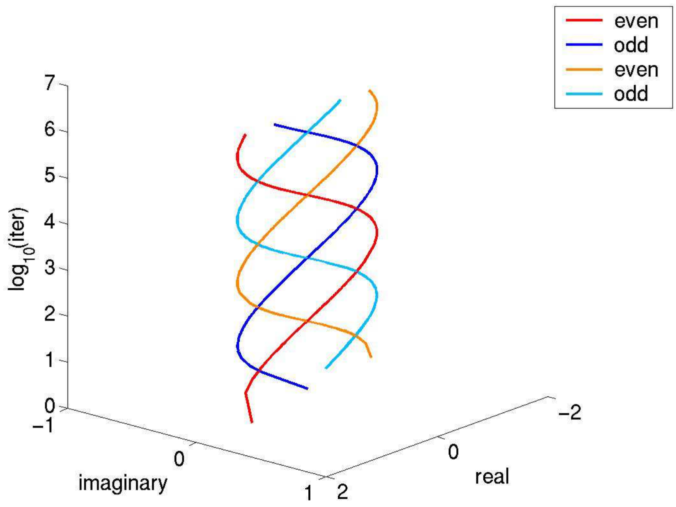

Figure 3: The subtle four fold serpent

Analysis is easy given the following striking hypergeometric parametrization of (24) when $a = b \neq 0$, see [18], which was both *experimentally discovered* and is *computer provable*:

$$t_n(a, a) = \frac{1}{2}F_n(a) + \frac{1}{2}F_n(-a), \tag{25}$$

where

$$F_n(a) := -\frac{a^n 2^{1-\omega}}{\omega\,\beta(n+\omega, -\omega)}\,{}_2\mathrm{F}_1\left(\omega, \omega; n+1+\omega; \frac{1}{2}\right).$$

Here

$$\beta(n+1+\omega, -\omega) := \frac{\Gamma\,(n+1)}{\Gamma\,(n+1+\omega)\,\Gamma\,(-\omega)}, \text{ and } \omega := \frac{1-1/a}{2}.$$

Indeed, once (25) was discovered by a combination of insight and methodical computer experiment, its proof is highly representative of the changing paradigm: both sides satisfy the same recursion and the same initial conditions. This can be checked in *Maple* and if one looks inside the computation, one learns which *confluent hypergeometric identities* are needed for an explicit human proof.

As noted, study of $\mathcal{R}$ devolved to *hard but compelling* conjectures on complex dynamics, with many interesting *proven* and *unproven* generalizations. In [23] consideration is made of continued fractions like

$$\mathcal{S}_1(a) = \cfrac{1^2 a_1^2}{1 + \cfrac{2^2 a_2^2}{1 + \cfrac{3^2 a_3^2}{1 + \ddots}}}$$

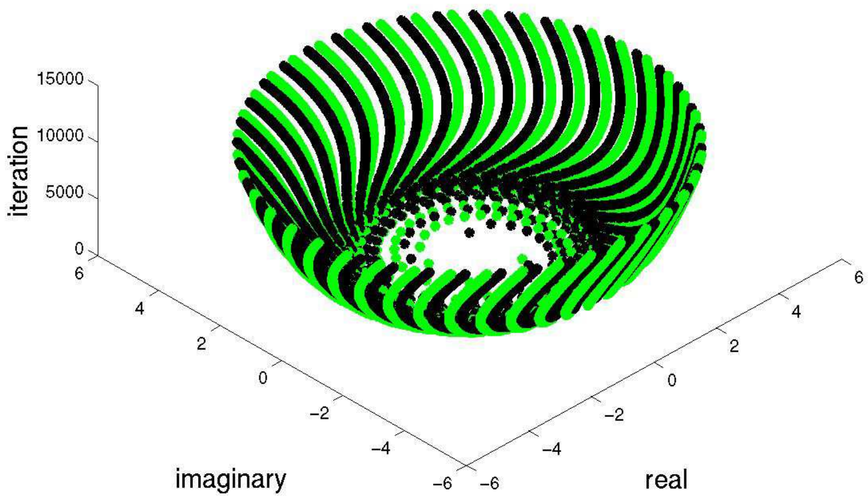

Figure 4: A period three dynamical system
(odd and even iterates)

for *any* sequence $a \equiv (a_n)_{n=1}^{\infty}$ and convergence properties obtained for deterministic and random sequences (a_n). For the deterministic case the best results obtained are for periodic sequences, satisfying $a_j = a_{j+c}$ for all j and some finite c. The dynamics are considerably more varied, as illustrated in Figure 4.

9 Coincidence and Fraud

Coincidences do occur, and such examples drive home the need for reasonable caution in this enterprise. For example, the approximations

$$\pi \;\approx\; \frac{3}{\sqrt{163}}\log(640320), \qquad \pi \;\approx\; \sqrt{2}\,\frac{9801}{4412}$$

occur for deep number theoretic reasons—the first good to 15 places, the second to eight. By contrast

$$e^{\pi} - \pi \;=\; \mathbf{19.999099979}189475768\ldots$$

most probably for no good reason. This seemed more bizarre on an eight digit calculator. Likewise, as spotted by Pierre Lanchon recently,

$$e \;=\; \overline{\mathbf{10.10110111111000010}}101000101100\ldots$$

while

$$\pi \;=\; 11.0010\overline{\mathbf{0100001111110110101}}01000\ldots$$

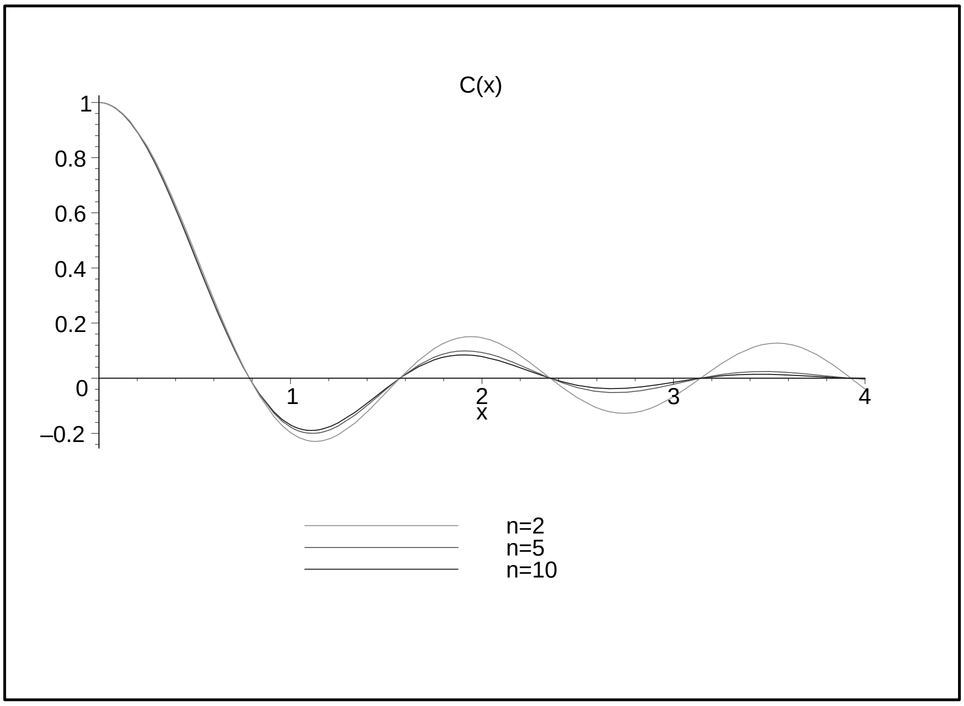

Figure 5: First few terms of $\prod_{n\geq 1} \cos(x/k)$

have 19 bits agreeing in base two—with one read right to left. More extended coincidences are almost always contrived, as illustrated by the following:

$$\sum_{n=1}^{\infty} \frac{[n \tanh(\pi/2)]}{10^n} \approx \frac{1}{81}, \qquad \sum_{n=1}^{\infty} \frac{[n \tanh(\pi)]}{10^n} \approx \frac{1}{81}.$$

The first holds to **12** decimal places, while the second holds to **268** places. This phenomenon can be understood by examining the continued fraction expansion of the constants $\tanh(\pi/2)$ and $\tanh(\pi)$: the integer **11** appears as the third entry of the first, while **267** appears as the third entry of the second.

Bill Gosper, commenting on the extraordinary effectiveness of continued-fraction expansions to "see" what is happening in such problems, declared "It looks like you are cheating God somehow."

A fine illustration is the unremarkable decimal $\alpha = 1.4331274267223117583\ldots$ whose continued fraction begins $[1, 2, 3, 4, 5, 6, 7, 8, 9\ldots]$ and so most probably is a ratio of Bessel functions. Indeed $I_0(2)/I_1(2)$ was what generated the decimal. Similarly, π and e are quite different as continued fractions, less so as decimals.

A more sobering example of high-precision "fraud" is the integral

$$\pi_2 := \int_0^{\infty} \cos(2x) \prod_{n=1}^{\infty} \cos\left(\frac{x}{n}\right) dx. \tag{26}$$

The computation of a high-precision numerical value for this integral is rather challenging, due in part to the oscillatory behavior of $\prod_{n\geq 1}\cos(x/n)$ (see Figure 2), but mostly due to the difficulty of computing high-precision evaluations of the integrand function. Note that evaluating thousands of terms of the infinite product would produce only a few correct digits. Thus it is necessary to rewrite the integrand function in a form more suitable for computation. This can be done by writing

$$f(x) = \cos(2x)\left[\prod_{1}^{m}\cos(x/k)\right]\exp(f_m(x)), \tag{27}$$

where we choose $m > x$, and where

$$f_m(x) = \sum_{k=m+1}^{\infty}\log\cos\left(\frac{x}{k}\right). \tag{28}$$

The log cos evaluation can be expanded in a Taylor series [1, pg 75], as follows:

$$\log\cos\left(\frac{x}{k}\right) = \sum_{j=1}^{\infty}\frac{(-1)^j 2^{2j-1}(2^{2j}-1)B_{2j}}{j(2j)!}\left(\frac{x}{k}\right)^{2j},$$

where B_{2j} are *Bernoulli numbers*. Note that since $k > m > x$ in (28), this series converges. We can now write

$$\begin{aligned} f_m(x) &= \sum_{k=m+1}^{\infty}\sum_{j=1}^{\infty}\frac{(-1)^j 2^{2j-1}(2^{2j}-1)B_{2j}}{j(2j)!}\left(\frac{x}{k}\right)^{2j} \\ &= -\sum_{j=1}^{\infty}\frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}}\left[\sum_{k=m+1}^{\infty}\frac{1}{k^{2j}}\right]x^{2j} \\ &= -\sum_{j=1}^{\infty}\frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}}\left[\zeta(2j)-\sum_{k=1}^{m}\frac{1}{k^{2j}}\right]x^{2j}. \end{aligned}$$

This can now be written in a compact form for computation as

$$f_m(x) = -\sum_{j=1}^{\infty}a_j b_{j,m}x^{2j}, \tag{29}$$

where

$$a_j = \frac{(2^{2j}-1)\zeta(2j)}{j\pi^{2j}} \qquad b_{j,m} = \zeta(2j)-\sum_{k=1}^{m}1/k^{2j}. \tag{30}$$

Computation of these b coefficients must be done to a much higher precision than that desired for the quadrature result, since two very nearly equal quantities are subtracted here.

The integral can now be computed using, for example, the tanh-sinh quadrature scheme. The first 60 digits of the result are the following:

$$0.392699081698724154807830422909937860524645434187231595926812\ldots$$

At first glance, this appears to be $\pi/8$. But a careful comparison with a high-precision value of $\pi/8$, namely

$$0.392699081698724154807830422909937860524646174921888227621868\ldots$$

reveals that they are *not* equal—the two values differ by approximately 7.407×10^{-43}. Indeed, these two values are provably distinct. The reason is governed by the fact that $\sum_{n=1}^{55} 1/(2n+1) > 2 > \sum_{n=1}^{54} 1/(2n+1)$. See [16, Chap. 2] for additional details.

A related example is the following. Recall the *sinc* function

$$\operatorname{sinc}(x) \ := \ \frac{\sin x}{x}.$$

Consider, the seven highly oscillatory integrals below.

$$\begin{aligned}
I_1 &:= \int_0^\infty \operatorname{sinc}(x)\, dx \ = \ \frac{\pi}{2}, \\
I_2 &:= \int_0^\infty \operatorname{sinc}(x)\operatorname{sinc}\left(\frac{x}{3}\right)\, dx \ = \ \frac{\pi}{2}, \\
I_3 &:= \int_0^\infty \operatorname{sinc}(x)\operatorname{sinc}\left(\frac{x}{3}\right)\operatorname{sinc}\left(\frac{x}{5}\right)\, dx \ = \ \frac{\pi}{2}, \\
&\ddots \\
I_6 &:= \int_0^\infty \operatorname{sinc}(x)\operatorname{sinc}\left(\frac{x}{3}\right)\cdots\operatorname{sinc}\left(\frac{x}{11}\right)\, dx \ = \ \frac{\pi}{2}, \\
I_7 &:= \int_0^\infty \operatorname{sinc}(x)\operatorname{sinc}\left(\frac{x}{3}\right)\cdots\operatorname{sinc}\left(\frac{x}{13}\right)\, dx \ = \ \frac{\pi}{2}.
\end{aligned}$$

However,

$$\begin{aligned}
I_8 &:= \int_0^\infty \operatorname{sinc}(x)\operatorname{sinc}\left(\frac{x}{3}\right)\cdots\operatorname{sinc}\left(\frac{x}{15}\right)\, dx \\
&= \frac{467807924713440738696537864469}{935615849440640907310521750000}\pi \approx 0.499999999992646\pi.
\end{aligned}$$

When this was first found by a researcher, using a well-known computer algebra package, both he and the software vendor concluded there was a "bug" in the software. Not so! It is easy to see that the limit of these integrals is $2\,\pi_1$, where

$$\pi_1 := \int_0^\infty \cos(x) \prod_{n=1}^{\infty} \cos\left(\frac{x}{n}\right)\, dx. \tag{31}$$

This can be seen via *Parseval's theorem*, which links the integral

$$I_N := \int_0^\infty \operatorname{sinc}(a_1 x)\operatorname{sinc}(a_2 x)\cdots\operatorname{sinc}(a_N x)\, dx$$

with the volume of the polyhedron P_N given by

$$P_N := \{x : |\sum_{k=2}^{N} a_k x_k| \le a_1, |x_k| \le 1, 2 \le k \le N\},$$

where $x := (x_2, x_3, \cdots, x_N)$. If we let

$$C_N := \{(x_2, x_3, \cdots, x_N) : -1 \le x_k \le 1, 2 \le k \le N\},$$

then

$$I_N = \frac{\pi}{2a_1}\frac{\operatorname{Vol}(P_N)}{\operatorname{Vol}(C_N)}.$$

Thus, the value drops precisely when the constraint $\sum_{k=2}^{N} a_k x_k \le a_1$ becomes *active* and bites the hypercube C_N. That occurs when $\sum_{k=2}^{N} a_k > a_1$. In the above, $\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{13} < 1$, but on addition of the term $\frac{1}{15}$, the sum exceeds 1, the volume drops, and $I_N = \frac{\pi}{2}$ no longer holds. A similar analysis applies to π_2. Moreover, it is fortunate that we began with π_1 or the falsehood of the identity analogous to that displayed above would have been much harder to see.

10 Further Directions and Implications

In spite of the examples of the previous section, it must be acknowledged that computations can in many cases provide very compelling evidence for mathematical assertions. As a single example, recently Yasumasa Kanada of Japan calculated π to over one trillion decimal digits (and also to over one trillion hexadecimal digits). Given that such computations, which take many hours on large, state-of-the-art supercomputers, are prone to many types of error, including hardware failures, system software problems, and especially programming bugs, how can one be confident in such results?

In Kanada's case, he first used two different arctangent-based formulas to evaluate π to over one trillion hexadecimal digits. Both calculations agreed that the hex expansion beginning at position 1,000,000,000,001 is `B4466E8D21 5388C4E014`. He then applied a variant of the BBP formula for π, mentioned in Section 3, to calculate these hex digits directly. The result agreed exactly. Needless to say, it is exceedingly unlikely that three different computations, each using a completely distinct computational approach, would all perfectly agree on these digits, unless all three are correct.

Another, much more common example is the usage of probabilistic primality testing schemes. Damgard, Landrock and Pomerance showed in 1993 that if an integer n has k bits, then the probability that it is prime, provided it passes the most commonly used probabilistic test, is greater than $1 - k^2 4^{2-\sqrt{k}}$, and for certain k is even higher [25]. For instance, if n has 500 bits, then this probability is greater than $1 - 1/4^{28m}$. Thus a 500-bit integer that passes this test even once is prime with prohibitively safe odds—the chance of a false declaration of primality is less than one part in Avogadro's number (6×10^{23}). If it passes the test for four pseudo-randomly chosen integers a, then the chance of false declaration of primality is less than one part in a googol (10^{100}). Such probabilities are many orders of magnitude more remote than the chance that an undetected hardware or software error has occurred in the computation. Such methods thus draw into question the distinction between a probabilistic test and a "provable" test.

Another interesting question is whether these experimental methods may be capable of discovering facts that are fundamentally beyond the reach of formal proof methods, which, due to Gödel's result, we know must exist; see also [24].

One interesting example, which has arisen in our work, is the following. We mentioned in Section 3 the fact that the question of the 2-normality of π reduces to the question of whether the chaotic iteration $x_0 = 0$ and

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

where $\{\cdot\}$ denotes fractional part, is equidistributed in the unit interval.

It turns out that if one defines the sequence $y_n = \lfloor 16x_n \rfloor$ (in other words, one records which of the 16 subintervals of $(0, 1)$, numbered 0 through 15, that x_n lies in), that the sequence (y_n), when interpreted as a hexadecimal string, appears to precisely generate the hexadecimal digit expansion of π. We have checked this to 1,000,000 hex digits and have found no discrepancies. It is known that (y_n) is a very good approximation to the hex digits of π, in the sense that the expected value of the number of errors is finite [15, Section 4.3] [11]. Thus one can argue, by the second Borel-Cantelli lemma, that in a heuristic sense the probability that there is any error among the remaining digits after the first million is less than 1.465×10^{-8} [15, Section 4.3]. Additional computations could be used to lower this probability even more.

Although few would bet against such odds, these computations do not constitute a rigorous proof that the sequence (y_n) is identical to the hexadecimal expansion of π. Perhaps some day someone will be able to prove this observation rigorously. On the other hand, maybe not—maybe this observation is in some sense an "accident" of mathematics, for which no proof will ever be found. Perhaps numerical validation is all we can ever achieve here.

11 Conclusion

We are only now beginning to digest some very old ideas:

> *Leibniz's idea is very simple and very profound. It's in section VI of the Discours [de métaphysique]. It's the observation that the concept of law becomes vacuous if arbitrarily high mathematical complexity is permitted, for then there*

Figure 6: Advanced Collaborative Environment in Vancouver

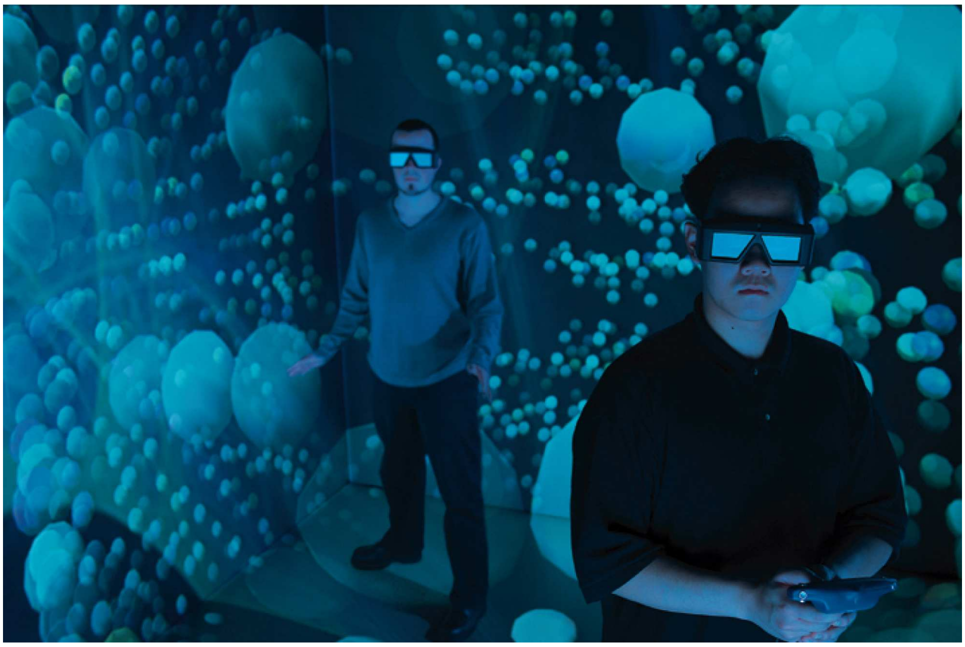

Figure 7: Polyhedra in an Immersive Environment

is always a law. Conversely, if the law has to be extremely complicated, then the data is irregular, lawless, random, unstructured, patternless, and also incompressible and irreducible. A theory has to be simpler than the data that it explains, otherwise it doesn't explain anything. Gregory Chaitin [24]

Chaitin argues convincingly that there are many mathematical truths which are logically and computationally irreducible—they have *no good reason* in the traditional rationalist sense. This in turn adds force to the desire for evidence even when proof may not be possible. Computer experiments can provide precisely the sort of evidence that is required.

Although computer technology had its roots in mathematics, the field is a relative latecomer to the application of computer technology, compared say with physics and chemistry. But now this is changing, as an army of young mathematicians, many of whom have been trained in the usage of sophisticated computer math tools from their high school years, begin their research careers. Further advances in software, including compelling new mathematical visualization environments (see Figures 6 and 7), will have their impact. And the remarkable trend towards greater miniaturization (and corresponding higher power and lower cost) in computer technology, as tracked by Moore's Law, is pretty well assured to continue for at least another ten years, according to Gordon Moore himself and other industry analysts. As Richard Feynman noted back in 1959, "There's plenty of room at the bottom." [27]. It will be interesting to see what the future will bring.

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