Experimental Mathematics: Examples, Methods and Implications

David H. Bailey and Jonathan M. Borwein

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]

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 timesaver 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 editions are far more expansive, robust, and user-friendly than when they first appeared twenty to twenty-five years ago. But numerous other tools, some of which emerged only 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`; (4) the electronic geometry site at `http://www.eg-models.de`; and numerous others. See

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

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

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 forty 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 twelve 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 researL)”SKads Glvuwp“”s“NB7M–öBLnLreseauwp“”sof this Karp’”BKof GhCLLLreseauwi.dEeLB;)KbuBL 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: "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 a PSLQ program, that

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

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

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

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, 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

$$\prod_{m=1}^{M} (b^m - i)$$

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, p. 77]. Further details on these results are given in [15, Sec. 4.3], [6], [12].

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, Borwein 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 nonzero 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

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

Evaluating this in EZFace+, we quickly obtain

$$S_{2,3} = 0.15616693338117691588103590968798819368577670984030387295752935449707503744029579145520565370935814757 8\ldots.$$

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: π^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:

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

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:

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

On the other hand, a general proof of

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

remains elusive. There has been abundant evidence amassed to support the conjectured identity (19) since it was discovered experimentally in 1996. The first eighty-five instances of (19) were recently affirmed in calculations by Petr Lisoněk 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 that sheds no light on (19) (see [21]).

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 that are also well suited for parallel processing [13], [14], [16, p. 312]. These schemes are based on the *Euler-Maclaurin summation* formula [3, p. 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

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

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 $h > 0$,

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

where $x_j = g(hj)$ and $w_j = g'(hj)$ are abscissas and weights that can be precomputed. 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

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

Here $G = \sum_{k\geq 0}(-1)^k/(2k+1)^2$ 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:

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

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

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

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:

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

where

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

The "identity" (21) has been verified to over 5000 decimal digit accuracy, but a proof is not yet known. It arises from the volume of an ideal tetrahedron in hyperbolic space, [15, pp. 90–1]. 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

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

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

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

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

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

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

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: $0.693\ldots$. 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 $0 < b < a$,

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

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

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

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

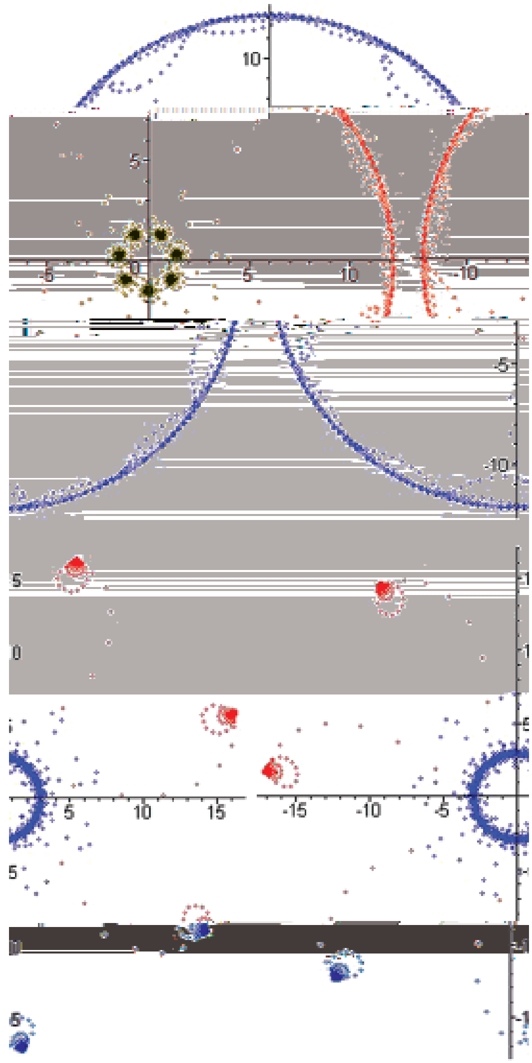

Figure 2. Dynamics and attractors of various iterations.

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

Indeed, it follows (see [19]) that

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

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

$$\mathcal{R}_1\left(\frac{1}{4\pi}\beta\left(\frac14,\frac14\right), \frac{\sqrt{2}}{8\pi}\beta\left(\frac14,\frac14\right)\right) = \frac12 \sum_{n\in\mathbf{Z}} \frac{\operatorname{sech}(n\pi)}{1+n^2}$$

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

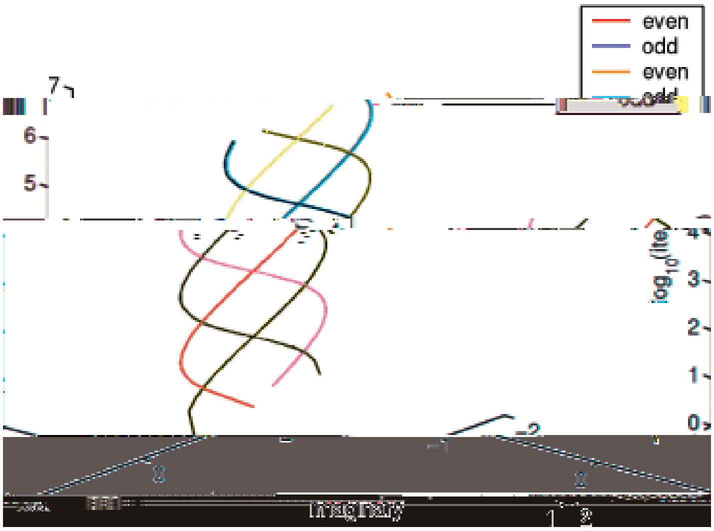

Figure 3. The subtle fourfold serpent.

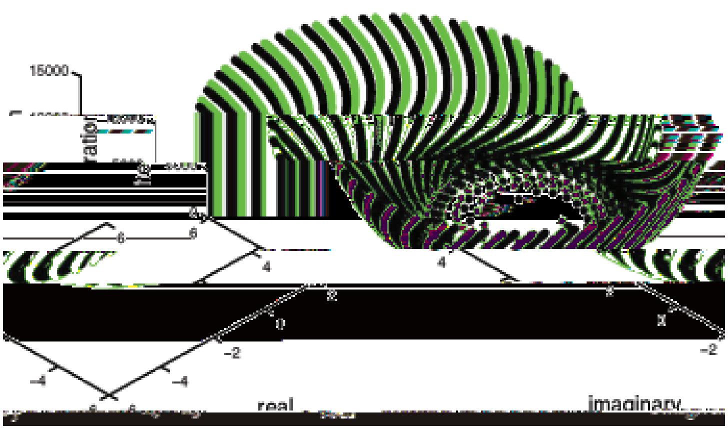

Figure 4. A period three dynamical system (odd and even iterates).

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

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 based only 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 structures appear; see Figure 2. With assistance of such plots, the behavior of these iterates (and the Ramanujan continued fractions) is 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 $\theta := \arg\Gamma((1+i)/2)$.

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

$$F_n(a) := -\frac{a^n 2^{1-\omega}}{\omega\,\beta(n+\omega,-\omega)}\,{}_2F_1\left(\omega,\omega;n+1+\omega;\frac{1}{2}\right).$$

Here

$$\beta(n+1+\omega,-\omega) := \frac{\Gamma(n+1)}{\Gamma(n+1+\omega)\Gamma(-\omega)}, \quad \text{and}$$

$$\omega := \frac{1-1/a}{2}.$$

Indeed, once (25) was discovered by a combination of insight and methodical computer experiment, its proof became 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

$$S_1(a) = \cfrac{1^2a_1^2}{1 + \cfrac{2^2a_2^2}{1 + \cfrac{3^2a_3^2}{1 + \ddots}}}$$

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.

Coincidence and Fraud

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

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

occur for deep number theoretic reasons: the first good to fifteen 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

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

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

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

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

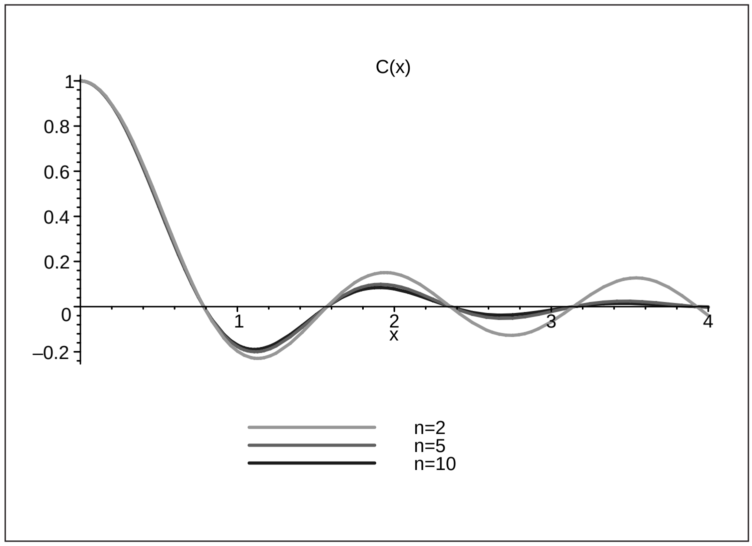

Figure 5. First few terms of $\prod_{n\geq 1}\cos(x/k)$.

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, p. 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

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

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 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 pseudorandomly 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, are 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, 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

Figure 7. Polyhedra in an immersive environment.

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 someday 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.

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 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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