EXPLORATORY EXPERIMENTATION AND COMPUTATION

1. Exploratory Experimentation

I believe our research community is facing a great challenge to re-evaluate the role of proof in light of the growing power of current computer systems, of modern mathematical computing packages, and of the growing capacity to data-mine on the Internet. Add to that the enormous complexity of many modern capstone results such as the Poincaré conjecture, Fermat's last theorem, and the Classification of finite simple groups. As the need and prospects for inductive mathematics blossom, the requirement to ensure the role of proof is properly founded remains undiminished.

I share with George Polya (1887-1985) the view that while learned, *"intuition comes to us much earlier and with much less outside influence than formal arguments"* [12, 2 p. 128]. Polya went on to reaffirm, nonetheless, that proof should certainly be taught in school. I turn to observations, many of which have been fleshed out in my recently coauthored books *The Computer as Crucible* [7], *Mathematics by Experiment* [5], and *Experimental Mathematics in Action* [3]. I want to argue for the changing nature of mathematical knowledge and in consequence to ask questions such as "How do we come to believe and trust pieces of mathematics?", "Why do we wish to prove things?" and "How do we teach what and why to students?"

I like various notions of embodied cognition. Smail [14, p. 113] writes: "*the large human brain evolved over the past 1.7 million years to allow individuals to negotiate the growing complexities posed by human social living.*" We find various modes of argument more palatable than others, and are more prone to make certain kinds of errors than others. Likewise, Steve Pinker's observation about language [11, p. 83] as founded on *". . . the ethereal notions of space, time, causation, possession, and goals that appear to make up a language of thought."* This remains so within mathematics. The computer offers scaffolding both to enhance mathematical reasoning, as with the computation with E_8, and to restrain mathematical error.

1.1. **Experimental mathodology.**

We start [7] with Justice Potter Stewart's famous 1964 comment on pornography: *"I know it when I see it."* A bit less informally, by *experimental mathematics* I intend: (i) Gaining insight and *intuition*; (ii) *Discovering* new relationships; (iii) *Visualizing*

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math principles; (iv) *Testing* and especially *falsifying* conjectures; (v) *Exploring* a possible result to see if it *merits* formal proof; (vi) *Suggesting* approaches for formal proof; (vii) *Computing* replacing lengthy hand derivations; (viii) *Confirming* analytically derived results [5]. Of these the first five play a central role and the sixth a most significant one for me, but connotes computer-assisted or computer-directed proof and is quite far from *Formal Proof* as the topic of a special issue of these *Notices* in December 2008.

Giaquinto's attractive encapsulation: *"In short,* discovering *a truth is coming to believe it in an independent, reliable, and rational way"* [9, p. 50] has the satisfactory consequence that a student can discover results whether known to the teacher or not. Nor is it necessary to demand that each dissertation be original (only independently discovered).

Despite the conventional identification of mathematics with deductive reasoning, Kurt Gödel (1906-1978) in his 1951 Gibbs Lecture said: *"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."* He held this view until the end of his life despite–or perhaps because of—the epochal deductive achievement of his incompleteness results.

Also, one discovers that many great mathematicians from Archimedes and Galileo—who apparently said *"All truths are easy to understand once they are discovered; the point is to discover them."*—to Gauss, Poincaré, and Carleson have emphasized how much it helps to "know" the answer. Two millennia ago Archimedes wrote to Eratosthenes[1] *"For it is easier to supply the proof when we have previously acquired, by the method, some knowledge of the questions than it is to find it without any previous knowledge."* Think of the *Method* as an ur-precursor to today's interactive geometry software—with the caveat that, for example, *Cinderella* actually does provide certificates for much Euclidean geometry.

As 2006 Abel Prize winner Leonard Carleson describes in his 1966 ICM speech on his positive resolution of Luzin's 1913 conjecture (about the pointwise convergence of Fourier series for square-summable functions) after many years of seeking a counterexample he decided none could exist. The importance of this confidence is expressed as follows: *"The most important aspect in solving a mathematical problem is the conviction of what is the true result. Then it took 2 or 3 years using the techniques that had been developed during the past 20 years or so."*

By *digital assistance* I mean use of *artefacts* as: (s) *Modern Mathematical Computer Packages*—symbolic, numeric, geometric, or graphical. (ii) *Specialized Packages* or *General Purpose Languages* such as Fortran, C++, CPLEX, PARI, SnapPea, and MAGMA. (iii) *Web Applications* such as:

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[1] Introduction to his long-lost and recently re-constituted *Method of Mechanical Theorems.*

Sloane's Encyclopedia of Integer Sequences, the Inverse Symbolic Calculator,[2] Fractal Explorer, Jeff Weeks' Topological Games, or Euclid in Java.[3] (iv) *Web Databases* including Google, MathSciNet, ArXiv, Wikipedia, MathWorld , MacTutor, Amazon, and many more that are not always so viewed.

All entail *data-mining* in various forms. Franklin [8] argues Steinle's *"exploratory experimentation"* facilitated by *"widening technology"*, as in pharmacology, astrophysics, medicine, and biotechnology, is leading to a reassessment of what legitimates experiment; in that a "*local model*" is not now prerequisite. Hendrik Sørenson [15] cogently makes the case that *experimental mathematics*—as 'defined' above—is following similar tracks.

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

In consequence, boundaries between mathematics and the natural sciences and between inductive and deductive reasoning are blurred and getting more so. (See also [1].) I leave unanswered the philosophically-vexing if mathematically-minor question as to whether genuine *mathematical experiments* (as discussed in [5]) exist even if one embraces a fully idealist notion of mathematical existence. They sure feel like they do.

2. Pi, Partitions and Primes

I can not now imagine doing mathematics without a computer nearby. Characteristic or minimal polynomials, entirely abstract for me as a student, now are members of a rapidly growing box of concrete symbolic tools, as are many matrix decomposition results, the use of Groebner bases, Risch's decision algorithm for when an elementary function has an elementary indefinite integral, and so on. Many algorithmic components of a *computer algebra system* (CAS) are today extraordinarily effective when two decades ago they were more like 'toys'. This is equally true of extreme-precision calculation—a prerequisite for much of my own work [2, 6] and others [4]—or in combinatorics. As I will illustrate during the three decades that I have seriously tried to integrate computational experiment into my research, we have experienced at least a dozen *Moore's law* doublings. [5, 7][4]

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[2] Most of the functionality of the ISC is built into the "identify" function *Maple* starting with version 9.5. For example, `identify(4.45033263602792)` returns $\sqrt{3}+e$. As always, the experienced will extract more than the novice.

[3] A cross-section of such resources is available through `http://ddrive.cs.dal.ca/~isc/portal/` and `www.experimentalmath.info`.

[4] Combined with 1000 or more cpu's and fibre-optics, this leads to 6 or 7 orders of magnitude speed up for many Information Communication and Technology (ICT) functions.

2.1. **The partition function.** Consider the number of *additive partitions*, $p(n)$, of a natural number where we ignore order and zeroes. Now $5 = 4+1 = 3+2 = 3+1+1 = 2+2+1 = 2+1+1+1 = 1+1+1+1+1$, so $p(5) = 7$. The *ordinary generating function* (2.1) discovered by Euler is

$$\sum_{n=0}^{\infty} p(n)q^n \quad = \quad \prod_{k=1}^{\infty} \left(1-q^k\right)^{-1}. \tag{2.1}$$

(Use the geometric formula for $1/(1-q^k)$ and observe how powers of q^n occur.) The famous computation by MacMahon of $p(200) = 3972999029388$ if done *symbolically and entirely naively* from (2.1) on a reasonable laptop took 20 minutes in 1991, and about 0.17 seconds today while

$$p(2000) = 4720819175619413888601432406799959512200344166$$

took 2 minutes in 2009. Moreover, in December 2008, Crandall was able to calculate $p(10^9)$ in 3 seconds on his laptop, using the Hardy-Ramanujan-Rademacher 'finite' series for $p(n)$ along with FFT methods. Using such fast partition-number evaluation enabled Crandall to find *probable primes* $p(1000046356)$ and $p(1000007396)$. Each of these special partition numbers has roughly $35,000$ decimal digits. I have wondered when easy access to computation discourages innovation: would Hardy and Ramanujan have still discovered their marvellous formula for $p(n)$?

2.2. **Quartic algorithm for π.** Likewise, the record for computation of π has gone from under 29.37 million decimal digits, by Bailey in 1986 to over 1.649 trillion places by Takhashi in 2009. Since the algorithm below was used as part of each computation, it is interesting to compare the performance in each case: Set $a_0 := 6 - 4\sqrt{2}$ and $y_0 := \sqrt{2} - 1$. Iterate

$$y_{k+1} := \frac{1-(1-y_k^4)^{1/4}}{1+(1-y_k^4)^{1/4}}, \; a_{k+1} := a_k(1+y_{k+1})^4 - 2^{2k+3}y_{k+1}(1+y_{k+1}+y_{k+1}^2) \tag{2.2}$$

Then a_k converges *quartically* to $1/\pi$. Twenty full-precision iterations of (2.2), which was discovered on a 16K Radio Shack portable in 1983, produce an algebraic number that coincides with π to more than 1.7 trillion places. Together with the 1976 Salamin–Brent scheme (SB) [5, Ch. 3], (2.2) has been employed frequently over the past quarter century.

- **1986:** It took 28 hours to compute 29.36 million digits on 1 cpu of the then new CRAY-2 at NASA Ames using (2.2). Confirmation using another quadratic algorithm took 40 hours.[5]
- **2009:** On 1024 cores of a 2592 core *Appro Xtreme-X3* system 1.649 trillion digits via (SB) took 64 hours 14 minutes with 6732 GB of main memory, and (2.2) took 73 hours 28 minutes with 6348 GB of main memory.[6]

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[5] The computation uncovered hardware and software errors on the CRAY. Success required developing a speedup of the underlying FFT [5]. Now one can compute billions of digits of π on a desk top should one so wish.

[6] The two computations differed only in the last 139 places.

Daniel Shanks , who in 1961 computed π to over 100,000 digits, then told Phil Davis that a billion digit computation would be "forever impossible." But both Kanada and the Chudnovskys achieved that in 1989. Similarly, the intuitionists Brouwer and Heyting asserted the "impossibility" of ever knowing whether the sequence "0123456789" appears in the decimal expansion of π—it was found in 1997 by Kanada, beginning at position $17,387,594,880$.

2.3. **Euler's totient function ϕ.** As another measure of what changes over time and what doesn't, I consider two conjectures regarding $\phi(n)$, which counts the number of positive numbers less than and relatively prime to n.

2.3.1. **Giuga's conjecture (1950).** *An integer $n > 1$, is a prime if and only if* $\mathcal{G}_n := \sum_{k=1}^{n-1} k^{n-1} \equiv n-1 \mod n$. Counterexamples are necessarily *Carmichael numbers* (rare birds only proven infinite in 1994) and more. In [6, Ch. 5] we exploited that if a number $n = p_1 \cdots p_m$ with $m > 1$ prime factors p_i is a counterexample to Giuga's conjecture (i.e., satisfies $s_n \equiv n-1 \mod n$), then $p_i \neq p_j$, $\sum_{i=1}^{m} 1/p_i > 1$, and the primes form a *normal sequence*: $p_i \not\equiv 1 \mod p_j$ for $i \neq j$. This yielded enough structure, using some predictive experimentally-discovered heuristics, to build an efficient algorithm to show—over several months in 1995—that any counterexample had at least 3459 prime factors and so exceeded $10^{13,886}$, now extended to 10^{14164} in a 5 day desktop computation.[7] While writing this piece, I was able to obtain almost as good a bound of 3050 primes in under 110 minutes on my notebook and a bound of 3486 primes, and 14,000 digits, in under 14 hours.[8]

A harder related conjecture is:

2.3.2. **Lehmer's conjecture (1932).** $\phi(n)\big|(n-1)$ *if and only if n is prime.* He called this "*as hard as the existence of odd perfect numbers.*" Again, prime factors of counterexamples form a normal sequence, but now there is little extra structure. In a 1997 Simon Fraser M.Sc. thesis Erick Wong verified the conjecture for 14 primes, using normality and a mix of PARI, C^{++} and *Maple* to press the bounds of the 'curse of exponentiality. The related condition, $\phi(n) \mid (n+1)$, is known to have 8 solutions with no more than 7 factors: $2, F_0, \cdots, F_4$ (the *Fermat primes*), and a rogue pair: 4919055 and 6992962672132095, as confirmed by Wong, but 8 seems out of sight.

2.4. **Inverse computation and Apéry-like series.** Three ζ-formulae are

$$(\mathbf{a})\, \zeta(2) = 3\sum_{k=1}^{\infty} \frac{1}{k^2\binom{2k}{k}},\ (\mathbf{b})\, \zeta(3) = \frac{5}{2}\sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3\binom{2k}{k}},\ (\mathbf{c})\, \zeta(4) = \frac{36}{17}\sum_{k=1}^{\infty} \frac{1}{k^4\binom{2k}{k}} \quad (2.3)$$

Binomial identity (2.3)(a) has been known for two centuries, while (b)—exploited by Apéry in his 1978 proof of the irrationality of $\zeta(3)$—was discovered as early as 1890 by Markov, and (c) was noted by Comtet [3].

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[7] Our method fails after 8135 primes and my goal is someday to exhaust it.

[8] Using *Maple* not as before C^{++} which being compiled is orders-of-magnitude faster but in which the coding is much more arduous.

Using *integer relation methods,*[9] bootstrapping, and the "Pade" function (*Mathematica* and *Maple* both produce rational approximations well), in 1996 Dave Bradley and I [3, 6] found the following remarkable and unanticipated generating function for $\zeta(4n+3)$:

$$\sum_{k=0}^{\infty} \zeta(4k+3)\, x^{4k} \quad = \quad \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^3 \binom{2k}{k} (1 - x^4/k^4)} \prod_{m=1}^{k-1} \left(\frac{1 + 4x^4/m^4}{1 - x^4/m^4} \right) \qquad (2.4)$$

A decade later, following a quite analogous—but much more deliberate—experimental procedure, as detailed in [3], we were able to discover a similar general formula for $\zeta(2n+2)$ that is pleasingly parallel to (2.4):

$$\sum_{k=0}^{\infty} \zeta(2k+2)\, x^{2k} \quad = \quad 3 \sum_{k=1}^{\infty} \frac{1}{k^2 \binom{2k}{k} (1 - x^2/k^2)} \prod_{m=1}^{k-1} \left(\frac{1 - 4\, x^2/m^2}{1 - x^2/m^2} \right) \qquad (2.5)$$

When $x = 0$ we recover (2.3) (a) and (b). In 1996 we could reduce (2.4) to a finite form which we could not prove, but Almquist and Granville did a year later. A decade later Wilf-Zeilberger's algorithm, for which they were awarded the Steele Prize, could directly as implemented in *Maple* certify (2.5) [5, 3]. We found a comparable generating function for $\zeta(2n+4)$, giving(2.3) (c) when $x = 0$, but one for $\zeta(4n+1)$ elludes us.

2.5. **Reciprocal series for π.** Truly novel series for $1/\pi$, based on elliptic integrals, were discovered by Ramanujan around 1910. [3, 5, 16]. One is:

$$\frac{1}{\pi} \quad = \quad \frac{2\sqrt{2}}{9801} \sum_{k=0}^{\infty} \frac{(4k)!\,(1103 + 26390k)}{(k!)^4 396^{4k}}. \qquad (2.6)$$

Each term of (2.6) adds 8 correct digits. Gosper used (2.6) by the computation of a then-record 17 million digits of π in 1985—completing the first proof (2.6) [5, Ch. 3]. A little later David and Gregory Chudnovsky found the following variant, which lies in $Q(\sqrt{-163})$ rather than $Q(\sqrt{58})$:

$$\frac{1}{\pi} \quad = \quad 12 \sum_{k=0}^{\infty} \frac{(-1)^k\,(6k)!\,(13591409 + 545140134k)}{(3k)!\,(k!)^3\, 640320^{3k+3/2}}. \qquad (2.7)$$

Each term of (2.7) adds 14 correct digits. The brothers used it several times—culminating in a 1994 calculation to over four billion decimal digits. Their remarkable story was told in a prizewinning *New Yorker* article [13].

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[9] Named on of the top ten algorithms of the past century by *CISE* in 1999, these algorithms, (of which the most effective is Helaman Ferguson's *PSLQ* [5, 3]) find or exclude potential rational relations between vectors of real numbers.

A few years ago Jésus Guillera found various Ramanujan-like identities for π, using integer relation methods. The three most basic are:

$$\frac{4}{\pi^2} = \sum_{n=0}^{\infty}(-1)^n r(n)^5(13+180n+820n^2)\left(\frac{1}{32}\right)^{2n+1} \tag{2.8}$$

$$\frac{2}{\pi^2} = \sum_{n=0}^{\infty}(-1)^n r(n)^5(1+8n+20n^2)\left(\frac{1}{2}\right)^{2n+1} \tag{2.9}$$

$$\frac{4}{\pi^3} \overset{?}{=} \sum_{n=0}^{\infty} r(n)^7(1+14n+76n^2+168n^3)\left(\frac{1}{8}\right)^{2n+1}, \tag{2.10}$$

where $r(n) := (1/2 \cdot 3/2 \cdot \cdots \cdot (2n-1)/2)/n!$. Guillera proved (2.8) and (2.9) in tandem, using the *Wilf–Zeilberger algorithm* for formally proving hypergeometric-like identities [5, 3, 16] very ingeniously. No other proof is known and there seem to be no like formulae for $1/\pi^N$ with $N \geq 4$. The third (2.10) is certainly true,[10] but has no proof, nor does anyone have an inkling of how to prove it; especially as experiment suggests that it has no 'mate' unlike (2.8) and (2.9) [3]. My intuition is that if a proof exists it is more a verification than an explication and so I stopped looking. I am happy just to know the beautiful identity is true. [11] It may be so for no good reason. It might just have no proof and be a very concrete Gödel statement.

3. Concluding Remarks

The flood of information and tools in our information-soaked world is unlikely to abate. We have to learn and teach judgement when it comes to using what is possible digitally. This means mastering the sorts of techniques I have illustrated and having some idea why a software system does what it does. It also requires developing a curriculum which carefully teaches experimental computer-assisted mathematics.[12] Judith Grabner has noted that a large impetus for the development of modern rigor in mathematics came with the Napoleonic introduction of regular courses: lectures and text books force a precision and a codification that apprenticeship obviates. But it will never be the case that quasi-inductive mathematics supplants proof. We need to find a new equilibrium. That said, we are only beginning to tap new ways to enrich mathematics. formal proof engines. As Jacques Hadamard said [12]:

> "The object of mathematical rigor is to sanction and legitimize the conquests of intuition, and there was never any other object for it."

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[10] Guillera ascribes (2.10) to Gourevich, who used integer relation methods. I've just 'rediscovered' (2.10) using 30 digits, and checked it to 500 places in 10secs, 1200 in 6.25min, and 1500 in 25min: as a naive command-line instruction in *Maple*.

[11] Though it would be more remarkable were it eventually to fail.

[12] Such efforts are underway. I mention Victor Moll at Tulane, Marc Chamberland at Grinnell `www.math.grin.edu/~chamberl/courses/MAT444/syllabus.html`, Jan de Gier in Melbourne and Ole Warnaar at Univ. of Queensland.

Never have we had such a cornucopia of ways to generate intuition. The challenge is to learn how to harness them, how to develop and how to transmit the necessary theory and practice. The new Newcastle Priority Research Centre I direct, *CARMA*,[13] hopes to play a lead role in this endeavour.

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[13] **C**omputer **A**ssisted **R**esearch **M**athematics and its **A**pplications whose webpage is being developed at `www.newcastle.edu.au/research/centres/carmacentre.html`.