EXPLORATORY EXPERIMENTATION: DIGITALLY-ASSISTED DISCOVERY AND PROOF

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1. Exploratory Experimentation

Our community (appropriately defined) 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 mathematical 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 need to ensure the role of proof is properly founded remains undiminished. I share with Polya the view that

> *"[I]ntuition comes to us much earlier and with much less outside influence than formal arguments· · · Therefore, I think that in teaching (high school age youngsters we should emphasize intuitive insight more than, and long before, deductive reasoning."* — George Polya (1887-1985) [15, 2 p. 128]

He goes on to reaffirm, nonetheless, that proof should certainly be taught in school. I continue with some observations many of which have been fleshed out in my recent books *The Computer as Crucible* [7], *Mathematics by Experiment* [6], and *Experimental Mathematics in Action* [3]. My musings focus on the changing nature of mathematical knowledge and in consequence asks the 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 am persuaded by various notions of embodied cognition. Smail [16, p. 113] writes: "*[T]he large human brain evolved over the past 1.7 million years to allow individuals to negotiate the growing complexities posed by human social living.*" In consequence 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 [14, p. 83] as founded on *"...the ethereal notions of space, time, causation, possession, and goals that appear to make up a language of*

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This material is largely excerpted from a longer paper written for ICMI Study 19 "On Proof and Proving in Mathematics Education," and a plenary talk given in May 2009 at the corresponding Workshop at National Taiwan Normal University.

thought." remain equally potent within mathematics. The computer offers to provide scaffolding both to enhance mathematical reasoning and to restrain mathematical error.

To begin with let me briefly reprise what I mean by discovery, and by proof. The following attractive notion of *discovery* has the satisfactory consequence that a student can certainly discovery results whether known to the teacher or not. Nor is it necessary to demand that each dissertation be original (only independently discovered): *"In short, discovering a truth is coming to believe it in an independent, reliable, and rational way"*—Marcus Giaquinto [10, p. 50]. Next I shall take:

> **PROOF**,[1] n. a sequence of statements, each of which is either validly derived from those preceding it or is an axiom or assumption, and the final member of which, the conclusion, is the statement of which the truth is thereby established.

As for mathematics itself, I offer the following in which the term *proof* does not enter. Nor should it; mathematics is much more than proof alone:

> **MATHEMATICS**, n. a group of subjects, including algebra, geometry, trigonometry and calculus, concerned with number, quantity, shape, and space, and their inter-relationships, applications, generalizations and abstractions.
> **DEDUCTION**, n. the process of reasoning typical of mathematics and logic, in which a conclusion follows necessarily from given premises so that it cannot be false when the premises are true.
> **INDUCTION**, n. (Logic) a process of reasoning in which a general conclusion is drawn from a set of particular premises, often drawn from experience or from experimental evidence. The conclusion goes beyond the information contained in the premises and does not follow necessarily from them. $\cdots$ for example, large numbers of sightings at widely varying times and places provide very strong grounds for the falsehood that all swans are white.

It awaited the discovery of Australia to confound the seemingly compelling inductive conclusion that all swans are white. I observe that we typically take for granted the distinction between *induction* and *deduction* and rarely discuss their roles with either our colleagues or our students.

Despite the conventional identification of Mathematics with deductive reasoning, in his 1951 Gibbs Lecture Kurt Gödel (1906-1978) 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 the epochal

[1]All definitions are taken from the *Collin's Dictionary of Mathematics* which I co-authored. It is freely available within the MAA's digital mathematics library and commercially with Maple inside it at:
`www.mathresources.com/products/mathresource/index.html`

deductive achievement of his incompleteness results. Moreover, one discovers a substantial number of 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 Poincaré and Carleson have emphasized how much it helps to "know" the answer. Over two millennia ago Archimedes wrote to Eratosthenes in the introduction to his long-lost and recently re-constituted *Method of Mechanical Theorems* [12]

> *"For some things, which first became clear to me by the mechanical method, were afterwards proved geometrically, because their investigation by the said method does not furnish an actual demonstration.* 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 counter-example 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."*

I will now assume that all proofs discussed are "non-trivial" in some fashion—since the issue of using inductive methods is really only of interest with this caveat. Armed with these terms, it remains to say that by *digital assistance* I intend the use of such *artefacts* as:

1. *Modern Mathematical Computer Packages*—be they Symbolic, Numeric, Geometric, or Graphical. I would classify all of these as "modern hybrid workspaces". One might also envisage much more use of stereo visualization, haptic, and auditory devices.

2. *More Specialist Packages* or *General Purpose Languages* such as Fortran, C++, CPLEX, GAP, PARI, SnapPea, Graffiti, and MAGMA.

3. *Web Applications* such as: Sloane's Online Encyclopedia of Integer Sequences, the Inverse Symbolic Calculator, Fractal Explorer, Jeff Weeks' Topological Games, or Euclid in Java.[2]

4 *Web Databases* including Google, MathSciNet, ArXiv, Wikipedia, JSTOR, MathWorld, Planet Math, Digital Library of Mathematical Functions or (DLMF), MacTutor, Amazon, and many more sources that are not always viewed as part of the palette.

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[2]A cross-section of such resources are available through `http://ddrive.cs.dal.ca/~isc/portal/`.

All entail *data-mining* in various forms. Franklin [9] argues that what Steinle calls *"exploratory experimentation"* facilitated by *"widening technology"* as in pharmacology, astrophysics, biotechnology is leading to a reassessment of what is viewed as a legitimate experiment; in that a "*local model*" is not a prerequisite for a legitimate experiment. Hendrik Sørenson [17] cogently makes the case that *experimental mathematics*—as 'defined' below—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."*

Danny Hillis is quoted as saying recently that: *"Knowing things is very 20th century. You just need to be able to find things."* on how *Google* has already changed how we think.[3] This is clearly not yet true and will never be, yet it catches something of the changing nature of cognitive style in the 21st century. In consequence, the boundaries between mathematics and the natural sciences and between inductive and deductive reasoning are blurred and getting blurrier. This is discussed at some length by Jeremy Avigad [1].

1.1. **Experimental Mathodology.** We started [7] with Justice Potter Stewart's famous 1964 comment on pornography *"I know it when I see it."* I now reprise from [6] what we mean a bit less informally by *experimental mathematics*. Gaining insight and *intuition*; *Discovering* new relationships; *Visualizing* math principles; *Testing* and especially *falsifying* conjectures; *Exploring* a possible result to see if it *merits* formal proof; *Suggesting* approaches for formal proof; *Computing* replacing lengthy hand derivations; *Confirming* analytically derived results. Of these the first five play a central role and the sixth plays a significant one but refers to computer-assisted or computer-directed proof and is quite far from *Formal Proof* as the topic of a special issue of the *Notices of the AMS* in December 2008.

2. Mathematical Examples

I continue with various explicit examples. I leave it to the reader to decide how much frequently he or she wishes to exploit the processes I advertise.

2.1. **Example I: What Did the Computer Do?** In my own work computer experimentation and digitally-mediate research now invariably play a crucial part. (Even in seemingly non-computational areas of functional analysis and the like, there is frequently a computable consequence whose verification provides confidence in the result under development.) In a recent study of expectation or "box integrals" [4] we were able to evaluate a

[3]In Achenblog `http://blog.washingtonpost.com/achenblog/` of July 1 2008.

quantity, which had defeated us for years, namely

$$\mathcal{K}_1 := \int_3^4 \frac{\operatorname{arcsec}(x)}{\sqrt{x^2 - 4\,x + 3}}\,dx$$

in *closed-form* as

$$\begin{aligned}
\mathcal{K}_1 &= \mathrm{Cl}_2(\theta) - \mathrm{Cl}_2\left(\theta + \frac{\pi}{3}\right) - \mathrm{Cl}_2\left(\theta - \frac{\pi}{2}\right) + \mathrm{Cl}_2\left(\theta - \frac{\pi}{6}\right) - \mathrm{Cl}_2\left(3\,\theta + \frac{\pi}{3}\right) \qquad (2.1)\\
&+ \mathrm{Cl}_2\left(3\,\theta + \frac{2\pi}{3}\right) - \mathrm{Cl}_2\left(3\,\theta - \frac{5\pi}{6}\right) + \mathrm{Cl}_2\left(3\,\theta + \frac{5\pi}{6}\right) + \left(6\,\theta - \frac{5\,\pi}{2}\right)\log\left(2 - \sqrt{3}\right).
\end{aligned}$$

where $\mathrm{Cl}_2(\theta) := \sum_{n=1}^{\infty} \sin(n\theta)/n^2$ is the *Clausen function*, and

$$3\,\theta := \arctan\left(\frac{16 - 3\sqrt{15}}{11}\right) + \pi.$$

Along the way to the evaluation above, there were several stages of symbolic computation, including an expression for $\mathcal{K}_1$ with over 28,000 characters (perhaps 25 standard novel pages). It may well be that the closed form in (2.1) can be further simplified. In any event, the very satisfying process of distilling the computer's 28,000 character discovery, required a mixture of art and technology and I would be hard pressed to assert categorically whether it constituted a conventional proof. Nonetheless, it is correct and has been checked numerically to over a thousand-digit decimal precision. ■

I turn to an example I hope will reinforce my assertion that there is already an enormous amount to be mined on the internet. And this is before any mathematical character recognition tools have been made generally available and when it is still very hard to search mathematics on the web.

2.2. **Example II: What is That Number?** In 1995 or so Andrew Granville emailed me the number

$$\alpha := 1.4331274267223\ldots \qquad (2.2)$$

and challenged me to identify it; I think this was a test I could have failed. I asked *Maple* for its continued fraction. In the conventional concise notation I was rewarded with

$$\alpha = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, ...]. \qquad (2.3)$$

Even if you are unfamiliar with continued fractions, you will agree that the changed representation in (2.3) has exposed structure not apparent from (2.2)! I reached for a good book on continued fractions and found the answer $\alpha = I_1(2)/I_0(2)$ where I_0 and I_1 are *Bessel functions* of the first kind. Actually I remembered that all arithmetic continued fractions arise in such fashion, but as we shall see one now does not need to. In 2009 there are at least three "zero-knowledge" strategies: **1.** Given (2.3), type "arithmetic progression", "continued fraction" into *Google*; **2.** Type "1,4,3,3,1,2,7,4,2" into *Sloane's Encyclopaedia of Integer Sequences*;[4] **3.** Type the decimal

[4]See `http://www.research.att.com/~njas/sequences/`.

digits of α into the *Inverse Symbolic Calculator*.[5] I illustrate the results of each strategy.

1. The first three hits on typing "arithmetic progression", "continued fraction" into *Google* on Oct 15, 2008, are shown in Figure 1. Moreover, the MathWorld entry tells us that any arithmetic continued fraction is of a ratio of Bessel functions, as shown in the inset to Figure 1 which points to the second hit in Figure 1. The reader may wish to find which other search terms uncover the answer—perhaps in the newly unveiled *Wolfram Alpha*.

2. Typing the first few digits into Australian expat Sloane's interface yields

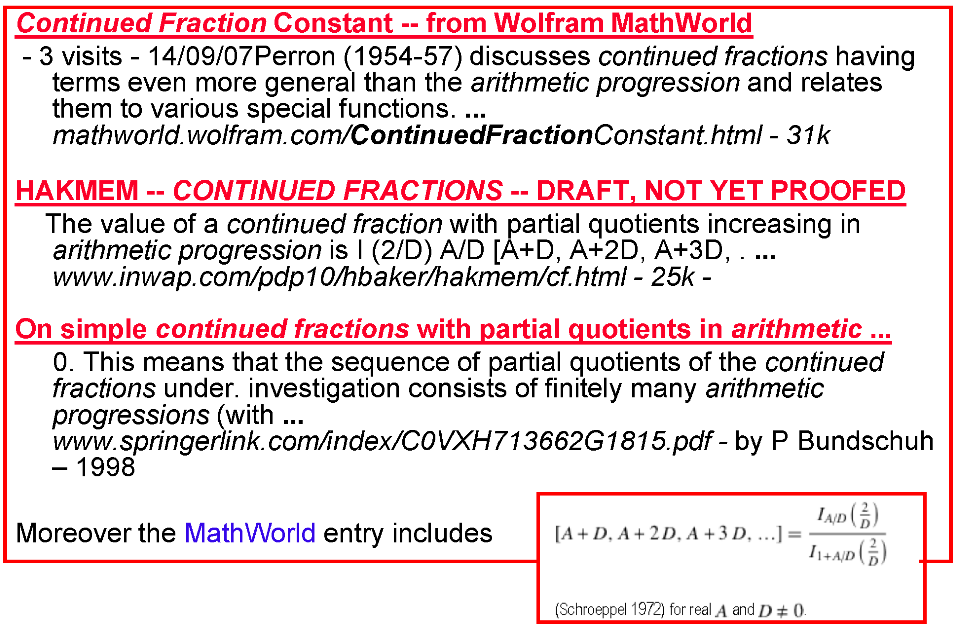


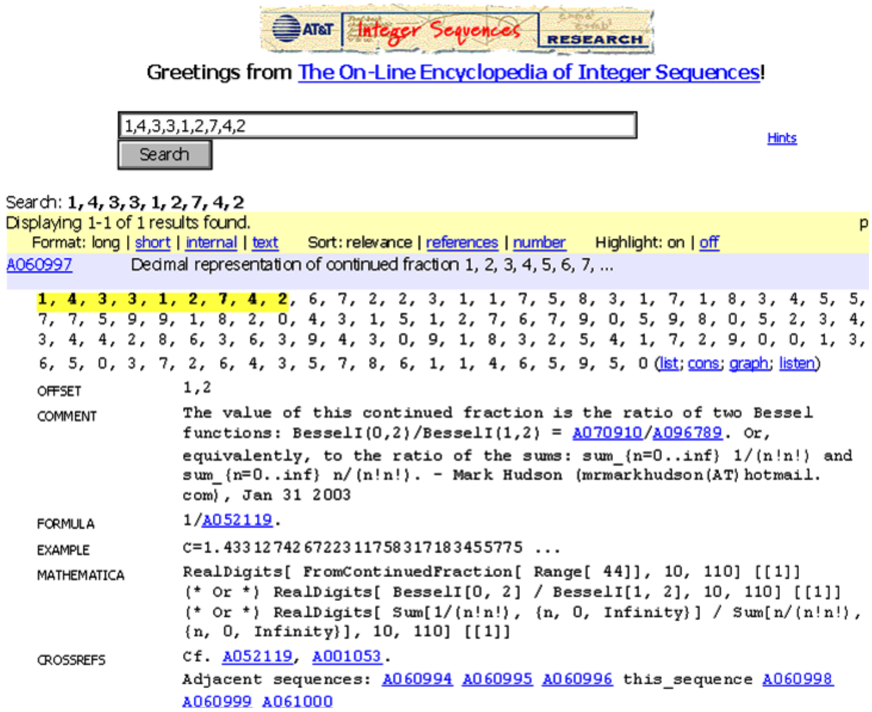
FIGURE 1. What Google and MathWorld offer.

Figure 2. In this case we are even told what the series representations of the requisite Bessel functions are, we are given sample code (in this case in *Mathematica*), and we are lead to many links and references. Moreover, the site is carefully moderated and continues to grow. This strategy became viable after May 14th 2008 when the sequence was added to the database—now with over 158,000 entries.

3. If one types the decimal for α into the Inverse Symbolic Calculator (ISC) it returns `Best guess: BesI(0,2)/BesI(1,2)`. ■

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.

[5]The online *Inverse Symbolic Calculator* `http://ddrive.cs.dal.ca/~isc` was newly web-accessible in 1995.


Greetings from The On-Line Encyclopedia of Integer Sequences!

1,4,3,3,1,2,7,4,2

Search

Hints

Search: **1, 4, 3, 3, 1, 2, 7, 4, 2**

Displaying 1-1 of 1 results found. p

Format: long | short | internal | text Sort: relevance | references | number Highlight: on | off

A060997 Decimal representation of continued fraction 1, 2, 3, 4, 5, 6, 7, ...

1, 4, 3, 3, 1, 2, 7, 4, 2, 6, 7, 2, 2, 3, 1, 1, 7, 5, 8, 3, 1, 7, 1, 8, 3, 4, 5, 5, 7, 7, 5, 9, 9, 1, 8, 2, 0, 4, 3, 1, 5, 1, 2, 7, 6, 7, 9, 0, 5, 9, 8, 0, 5, 2, 3, 4, 3, 4, 4, 2, 8, 6, 3, 6, 3, 9, 4, 3, 0, 9, 1, 8, 3, 2, 5, 4, 1, 7, 2, 9, 0, 0, 1, 3, 6, 5, 0, 3, 7, 2, 6, 4, 3, 5, 7, 8, 6, 1, 1, 4, 6, 5, 9, 5, 0 (list; cons; graph; listen)

OFFSET	1,2
COMMENT	The value of this continued fraction is the ratio of two Bessel functions: BesselI(0,2)/BesselI(1,2) = A070910/A096789. Or, equivalently, to the ratio of the sums: sum_{n=0..inf} 1/(n!n!) and sum_{n=0..inf} n/(n!n!). - Mark Hudson (mrmarkhudson(AT)hotmail.com), Jan 31 2003
FORMULA	1/A052119.
EXAMPLE	C=1.4331274267223117583171834557 75 ...
MATHEMATICA	RealDigits[FromContinuedFraction[Range[44]], 10, 110] [[1]] (* Or *) RealDigits[BesselI[0, 2] / BesselI[1, 2], 10, 110] [[1]] (* Or *) RealDigits[Sum[1/(n!n!), {n, 0, Infinity}] / Sum[n/(n!n!), {n, 0, Infinity}], 10, 110] [[1]]
CROSSREFS	Cf. A052119, A001053. Adjacent sequences: A060994 A060995 A060996 this_sequence A060998 A060999 A061000

FIGURE 2. What *Sloane's Encyclopaedia* offers.

2.3. **Example III: From Discovery to Proof.** The following was popularized in *Eureka*[6] in 1971.

$$0 < \int_0^1 \frac{(1-x)^4 x^4}{1+x^2}\, \mathrm{d}x \quad = \quad \frac{22}{7} - \pi \tag{2.4}$$

as described in [6]. The integrand is positive on $(0, 1)$ so the integral yields an area and $\pi < 22/7$. Set on a 1960 Sydney honours maths final exam[7] (2.4) perhaps originated in 1941 with the author of the 1971 article—Dalzeil who chose not reference his earlier self! Why should we trust this discovery? Well *Maple* and *Mathematica* both 'do it'. But this is *proof by appeal to authority* [11] and a better answer is to ask *Maple* for the indefinite integral

$$\int_0^{\mathbf{t}} \frac{(1-x)^4 x^4}{1+x^2}\, \mathrm{d}x \quad = \quad ?$$

The computer algebra system (CAS) will return

$$\int_0^t \frac{x^4\,(1-x)^4}{1+x^2} \mathrm{d}x \quad = \quad \frac{1}{7}\,t^7 - \frac{2}{3}\,t^6 + t^5 - \frac{4}{3}\,t^3 + 4\,t - 4\,\arctan(t)\,. \tag{2.5}$$

Finish by differentiating and using the Fundamental theorem of calculus. ■

[6]Eureka was an undergraduate Cambridge University journal.

[7]Alf van der Poorten recalls being shown this by Kurt Mahler in the mid-sixties.

This is probably not the proof one would find by hand, but it is rigorous, and represents an "instrumental use" of the computer. That a CAS will often be able to evaluate an indefinite integral or a finite sum whenever it can evaluate the corresponding definite integral or infinite sum frequently allows one to provide a certificate for such a discovery. In the case of a sum the certificate often takes the form of a mathematical induction. Another interesting feature of Example III is that it appears to be irrelevant that $22/7$ is the most famous continued-fraction approximation to π, as described by an expat Australian [13]. Not every discovery is part of a hoped-for pattern.

2.4. **Example IV: From Concrete to Abstract.** While studying *multiple zeta values* [6] we needed to show $M := A + B - C$ invertible, where the $n \times n$ matrices A, B, C respectively had entries

$$(-1)^{k+1}\binom{2\,n-j}{2\,n-k}, \quad (-1)^{k+1}\binom{2\,n-j}{k-1}, \quad (-1)^{k+1}\binom{j-1}{k-1} \tag{2.6}$$

So A and C are triangular while B is full. In six dimensions M is:

$$\begin{bmatrix} 1 & -22 & 110 & -330 & 660 & -924 \\ 0 & -10 & 55 & -165 & 330 & -462 \\ 0 & -7 & 36 & -93 & 162 & -210 \\ 0 & -5 & 25 & -56 & 78 & -84 \\ 0 & -3 & 15 & -31 & 35 & -28 \\ 0 & -1 & 5 & -10 & 10 & -6 \end{bmatrix}$$

After futilely peering at many cases i thought to ask *Maple* for the *minimal polynomial* of M :

```
> linalg[minpoly](M(12),t);
```

returns $-2 + t + t^2$. Emboldened I tried

```
> linalg[minpoly](B(20),t); linalg[minpoly](A(20),t);
  linalg[minpoly](C(20),t);
```

and was rewarded with $-1 + t^3, -1 + t^2, -1 + t^2$. A typical matrix has a full degree minimal polynomial, so we are assured that A, B, C really are roots of unity. Armed with this we are lead to try to prove

$$A^2 = I, \quad BC = A, \quad C^2 = I, \quad CA = B^2 \tag{2.7}$$

which is a nice combinatorial exercise (by hand or computer). Clearly then we obtain also

$$B^3 = B \cdot B^2 = B(CA) = (BC)A = A^2 = I \tag{2.8}$$

and $M^{-1} = \frac{M+I}{2}$ is again a fun exercise in formal algebra; as is confirming that we have discovered an amusing presentation of the symmetric group S_3. ■

Characteristic or minimal polynomials, entirely abstract for me as a student, now become members of a rapidly growing box of concrete symbolic tools, as do 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 CAS are 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, 4] and others [5]—or in combinatorics. The number of *additive partitions* of $n, p(n)$, has ordinary generating function $\prod_{k=1}^{\infty}(1-q^k)^{-1}$. On a reasonable laptop calculating $p(200) = 3972999029388$ naively from the o.g.f. took 20 minutes in 1991. Today it takes about 0.17 secs while $p(2000) = 4720819175619413888601432406799959512200344166$ takes two minutes naively and about 0.2 seconds using the built-in *Maple* recursion. Likewise, the record for computation of π has gone from under 30 million decimal digits in 1986 to over 1.6 trillion places this year.

3. Concluding Remarks

We live in an information-rich, judgement-poor world and the explosion of information and tools is not going to diminish. We have to learn and teach judgement when it comes to using what is already possible digitally. This means mastering the sorts of tools I have illustrated. But it will never be the case that quasi-inductive mathematics supplants proof. We need to find a new equilibrium. The following empirically-discovered identity

$$\begin{aligned} &\sum_{n=-\infty}^{\infty} \operatorname{sinc}(n)\operatorname{sinc}(n/3)\operatorname{sinc}(n/5)\cdots\operatorname{sinc}(n/23)\operatorname{sinc}(n/29) \qquad (3.1)\\ = &\int_{-\infty}^{\infty} \operatorname{sinc}(x)\operatorname{sinc}(x/3)\operatorname{sinc}(x/5)\cdots\operatorname{sinc}(x/23)\operatorname{sinc}(x/29)\,dx \end{aligned}$$

where the denumerators range over the odd primes. Provably, the following is true: The analogous "sum equals integral" identity remains valid for more than the first $10,176$ primes but stops holding after some larger prime, and thereafter the "sum less the integral" is positive but *much less than one part in a googolplex*. A stronger estimate is possible assuming the GRH [2].

That said, we are only beginning to scratch the surface of a very exciting set of tools for the enrichment of mathematics, not to mention the growing power of formal proof engines. I conclude with one of my favourite quotes from Jacques Hadamard [15]:

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

Never have we had such a cornucopia of fine tools 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*,[8] hopes to play a lead role in this endeavour.

[8]**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`.

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