High Performance Symbolic Computing: A Mathematician’s Perspective

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ABSTRACT. I intend to discuss such computation from a user’s perspective. Largely, using various of the zeta functions with which I have worked I will illustrate what is easy, what is hard, what is possible and what we aspire to be able to do. I will summarize some of the very demanding symbolic/numeric computations I have recently performed with David Broadhurst, Petr Lisoněk and others.

◊ And I will be rash enough* to give my own perspective on what needs to be done to bring symbolic computing into the 21st century — that is effectively using the parallel high performance systems of the next decade. In that context, I will also touch upon the Canadian Computational Collaboratory (www.c3.ca).

• A full HTML version follows later this fall (for MAA)

*At any rate verbally!
Overview and Disclaimers

- parallelism \equiv \text{more space/speed/stuff}

- exact \equiv \text{hybrid} = \text{symbolic/numeric}

- \textit{Goal}: Insight (demands speed = parallelism)
  - verification (""")
  - validations; proofs \textit{and} refutations
  - while HPC and HPN blur; with a merging of disciplines and collaborators
  - for analysis/algebra/geometry \& topology

- And now the examples \ldots

*“You shall soon gain the attention of those who count.” (A recent fortune cookie)*
A. Warmup

A.1: Some online quotes from *Empirical Mathematics*

1983: $\sqrt{2} - 1, \frac{\sqrt{3} - 1}{2}, \frac{\sqrt{5} - 1}{2}$: now ‘minpoly’ or “inverse calculator”

A.2: the “modular machine”.

1988-96: a cubic $\, _2F_1$. Consider

$$a := \sum_{m,n=-\infty}^{\infty} q^{m^2+mn+n^2},$$

$$b := \sum_{m,n=-\infty}^{\infty} \omega^{n-m} q^{n^2+mn+m^2},$$

where $\omega = e^{2\pi i/3}$ and

$$c := \sum_{m,n=-\infty}^{\infty} q^{(n+1/3)^2+(n+1/3)(m+1/3)+(m+1/3)^2}.$$
These three functions lie on the *Fermat curve*

\[ a^3 = b^3 + c^3 \]

and one has the lovely *cubic* parameterization of a hypergeometric function:

\[(1) \quad 2F1\left(\frac{1}{3}, \frac{2}{3}; 1; \frac{c^3}{a^3}\right) = a.\]

• In the modular world enough terms of a power series or a product are a *PROOF*.

• By 1996 (1) could be discovered and automated in Salvy et als’ GFUN.

**Coworkers:** Bailey, P. Borwein, Garvan, Lissoněk, Macdonald
A.3: MRI, 1997. Estimating high-resolution spectra from short data records makes maximum entropy reconstruction particularly important in multidimensional NMR where short records are unavoidable. The Hoch and Stern information measure, or neg-entropy, is defined in complex n–space by

$$H(X) = \sum_{j=1}^{n} h\left(\frac{X_j}{b}\right),$$

where $h$ is convex and defined (for $b$ a scaling factor) by

$$h(z) \triangleq |z| \ln \left(|z| + \sqrt{1 + |z|^2}\right) - \sqrt{1 + |z|^2}$$

- Our symbolic convex analysis package told me $h^*(z) = \cosh(|z|)$. (Shannon entropy: $x \ln x$–$x$ has conjugate exp($x$).)

◊ I’d never have tried by hand!

- Dual algorithms are now possible.

Coworkers: Marechal, Naugler, …, Fee
B. \( \pi \)

- Different forms/uses of parallelism:

**B.1: (Quartic algorithm.)** Set \( a_0 = 6 - 4\sqrt{2} \) and \( y_0 = \sqrt{2} - 1 \). Iterate

\[
y_{k+1} = \frac{1 - (1 - y_k^4)^{1/4}}{1 + (1 - y_k^4)^{1/4}} \\
a_{k+1} = a_k(1 + y_{k+1})^4 - 2^{2k+3}y_{k+1}(1 + y_{k+1} + y_{k+1}^2)
\]

Then \( a_k \) converges *quartically* to \( 1/\pi \).

- This, with the Salamin-Brent scheme, was used by Yasumasa Kanada in Tokyo in many computations of \( \pi \) over the past dozen years. In a 1997 computation, Kanada computed over 51 billion digits on a Hitachi supercomputer (18 iterations, 25 hrs on \( 2^{10} \) cpus); the present world record.

\( \diamond \) 50 billionth decimal digit of \( \pi \) or \( \frac{1}{\pi} \) is 042 ! And 0123456789 has appeared (Brouwer).
• Garvan and I found genuine \( \eta \)-based \( m \)-th order convergent approximations to \( \pi \) for any \( m \).

A nonic (ninth-order) algorithm follows. Set
\[
a_0 = 1/3, \quad r_0 = (\sqrt{3} - 1)/2, \quad s_0 = (1 - r_0^3)^{1/3}.
\]
Iterate
\[
\begin{align*}
t &= 1 + 2r_k \\
u &= [9r_k(1 + r_k + r_k^2)]^{1/3} \\
v &= t^2 + tu + u^2 \\
m &= \frac{27(1 + s_k + s_k^2)}{v} \\
a_{k+1} &= ma_k + 3^{2k-1}(1 - m) \\
s_{k+1} &= \frac{(1 - r_k)^3}{(t + 2u)v} \\
r_{k+1} &= (1 - s_k^3)^{1/3}
\end{align*}
\]

Then \( 1/a_k \) converges nonically to \( \pi \).
- These higher order algorithms are slower as computational schemes than the quartic algorithm. Though fewer iterations are required to achieve a given precision, each iteration is more expensive.

- Discovery of these methods involved enormous amounts of symbolic computation (‘Andrew’s $\prod \Rightarrow \sum$ algorithm’ etc.).

- Kanada’s estimate of time to run the same algorithm on a serial machine: “$\textit{infinite}$”.

**Coworkers:** Bailey, P. Borwein, Garvan, Kanada, Lisoněk
B.2: (‘pentium farming’ for binary digits.) Bailey, P. Borwein and Plouffe (1996) discovered a series for $\pi$ (and some other polylogarithmic constants) which allows one to compute hex–digits of $\pi$ without computing prior digits.

- The algorithm needs very little memory, does not need multiple precision and the running time grows only slightly faster than linearly in the order of the digit being computed.

The key, discovered using PSLQ, is: $\pi = \sum_{k=0}^{\infty} \left( \frac{1}{16} \right)^k \left( \frac{4}{8k + 1} - \frac{2}{8k + 4} - \frac{1}{8k + 5} - \frac{1}{8k + 6} \right)$.

They knew an algorithm would follow from such a formula and spent several months hunting for one.

Reverse Mathematical Engineering
• (Sept 97) Fabrice Bellard (INRIA) used a variant formula to compute 152 binary digits of \( \pi \), starting at the trillionth position \((10^{12})\). This took 12 days on 20 workstations working in parallel over the Internet.

• (Aug 98) Colin Percival (SFU, age 17) finished a similar computation of the five trillionth digit \((25 \text{ machines at about } 10 \times \text{the speed})\). Yielding in hex:

\[
07E45733CC790B5B5979.
\]

• In a series of inspired computations using *polylogarithmic ladders* Broadhurst has since found – and proved – similar identities for \( \zeta(3) \), \( \zeta(5) \) and Catalan’s constant \( G^* \).

**Coworkers:** BBP, Bellard, Broadhurst, Percival.

*Why \( G \) was missed?
\[ G := \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k + 1)^2} \quad (= L_{-4}(2)) \]

\[ = 3 \sum_{k=0}^{\infty} \frac{1}{2 \cdot 16^k} \left\{ \frac{1}{(8k + 1)^2} - \frac{1}{(8k + 2)^2} \right. \\
+ \frac{1}{2(8k + 3)^2} - \frac{1}{2^2(8k + 5)^2} \\
+ \frac{1}{2^2(8k + 6)^2} - \frac{1}{2^3(8k + 7)^2} \right\} \]

\[ -2 \sum_{k=0}^{\infty} \frac{1}{8 \cdot 16^{3k}} \left\{ \frac{1}{(8k + 1)^2} + \frac{1}{2(8k + 2)^2} \right. \\
+ \frac{1}{2^3(8k + 3)^2} - \frac{1}{2^6(8k + 5)^2} \\
- \frac{1}{2^7(8k + 6)^2} - \frac{1}{2^9(8k + 7)^2} \right\} \]

*His paper also gives some constants with ternary expansions.*
C. Normal families of primes

- High-level languages versus computational speed?

- A family of primes $\mathcal{P}$ is *normal* if it contains no primes $p, q$ such that $p$ divides $q - 1$.

  ◦ *Giuga’s conjecture* (1951) is that

  $$\sum_{k=1}^{n-1} k^{n-1} \equiv n - 1 \pmod{n}$$

  if and only if $n$ is prime.

  † *Agoh’s Conjecture* (1995) is equivalent:

  $$nB_{n-1} \equiv -1 \pmod{n} \iff n \text{ is prime.}$$

  ◦ *Lehmer’s conjecture* (1932) is that

  $$\phi(n) \mid n - 1$$

  if and only if $n$ is prime.
• Lehmer’s conjecture had been verified for up to 13 prime factors of \( n \), and we extended this to 14 prime factors. We also examined the related condition

\[
\phi(n) \mid n + 1
\]

which was known to have 8 solutions* with up to 6 prime factors (by Lehmer) and extended this to 7 prime factors.

• For all three of these conjectures the set of prime factors of any counterexample \( n \) is a normal family, and we exploited this property aggressively in our computations. But the next Lehmer cases (15 and 8) were way too large.

*2, \( F_0, \ldots, F_4 \) and a rogue pair: 4919055 and 6992962672132095.
• Any counterexample to the Giuga conjecture must be a *Carmichael number*; and an odd *Giuga number*: $n$ is squarefree and

$$\sum_{p|n} \frac{1}{p} - \prod_{p|n} \frac{1}{p} \in \mathbb{Z}.$$  

For example

$$\frac{1}{2} + \frac{1}{3} + \frac{1}{5} - \frac{1}{30} = 1.$$  

The largest we have found has 8 primes:

$$554079914617070801288578559178 = 2 \times 3 \times 11 \times 2331 \times 47059 \times 2259696349 \times 110725121051.$$  

• We tried to use up the only known branch-bound algorithm. Thirty lines of Maple became 2 months in C++ which crashed in Tokyo — but after confirming that $n$ has more than 13,800 digits.

**Coworkers:** D. Borwein, P. Borwein, Girgensohn, Wong and Wayne State Undergraduates
D. Khintchine and Ramanujan

- In different contexts different algorithms star.

D.1: The celebrated Khintchine constants $K_0$, $(K_{-1})$ – the limiting geometric (harmonic) mean of the elements of almost all simple continued fractions – have efficient Riemann zeta series; standard definitions are cumbersome products.

- The rational $\zeta$ series we used is: $\log K_0 \log 2 = 
\sum_{n=1}^{\infty} \frac{\zeta(2s) - 1}{s} \left(1 - \frac{1}{2} + \frac{1}{3} - \ldots + \frac{1}{2n-1}\right)$,
which accelerated and used with “recycling” evaluations of $\{\zeta(2s)\}$, gave us $K_0$ to thousands of digits.*

- Here

$\zeta(s) := \sum_{n=1}^{\infty} \frac{1}{n^s}$.

*From 7,350 digits it appears the Khintchine constant obeys its own prediction.
D.2: Computing $\zeta(N)$ (for $K-1$ odd $N$ are needed).

- $B_{2N} \equiv \zeta(2N)$ can be effectively computed (i) in parallel by *multi–sectioning* methods; or (ii) by FFT–enhanced *Newton (recycling) methods* on the series $\frac{\sinh}{\cosh}$.

- For $\zeta(2N + 1)$ we chose identities due to Ramanujan among others. Viz:

\[
\zeta(4N + 3) = -2 \sum_{k \geq 1} \frac{1}{k^{4N+3}(e^{2\pi k} - 1)} + \frac{2}{\pi} \left\{ \frac{4N + 7}{4} \zeta(4N+4) - \sum_{k=1}^{N} \zeta(4k)\zeta(4N+4-4k) \right\}
\]

\[
\zeta(4N + 1) = -\frac{2}{N} \sum_{k \geq 1} \frac{(\pi k + N)e^{2\pi k} - N}{k^{4N+1}(e^{2\pi k} - 1)^2} + \frac{1}{2N\pi} \left\{ (2N+1)\zeta(4N+2) + \sum_{k=1}^{2N} (-1)^k 2k\zeta(2k)\zeta(4N+2-2k) \right\}.
\]

*These have space advantages even as serial algorithms and work for poly-exp functions (Kevin Hare)
• Only a finite set of $\zeta(2N)$ values is required and the full precision value $e^\pi$ is reused throughout.*

• Very recently, I've decoded a “nicer” series for $\zeta(4N+1)$ from a few cases found by Plouffe with PSLQ. It is equivalent to:

$$\left\{2 - (-4)^{-N}\right\} \sum_{k=1}^{\infty} \frac{\coth(k\pi)}{k4N+1} - (-4)^{-2N} \sum_{k=1}^{\infty} \frac{\tanh(k\pi)}{k4N+1}$$

(3) \quad = Q_N \times \pi^{4N+1}

with $Q_N :=$

$$\sum_{k=0}^{2N+1} B_{4N+2-2k} B_{2k} \left\{(-4)^k + (-1)^k(k+1)/2(-4)^N 2^k\right\}$$

$$(4N+2-2k)!(2k)!$$

on substituting

$$\tanh(x) = 1 - \frac{2}{\exp(2x)+1} \quad \text{coth}(x) = 1 + \frac{2}{\exp(2x)-1}$$

and then solving for $\zeta(4N+1)$.

*The number $e^\pi$ is the easiest number to fast compute elliptically. One “differentiates” $e^{-s\pi}$ to obtain $\pi$. 
• Thus,

$$\zeta(5) = \frac{1}{294} \pi^5 +$$

$$\frac{2}{35} \sum_{k=1}^{\infty} \frac{1}{(1 + e^{2k\pi})k^5} + \frac{72}{35} \sum_{k=1}^{\infty} \frac{1}{(1 - e^{2k\pi})k^5}.$$

• Will we ever be able to identify universal formulae like (3) automatically? My solution was highly human assisted.

**Coworkers:** Bailey, Crandall, Hare, Plouffe.
E. Apéry and Riemann

- Parallelizable "bootlegged" discovery.

- Bradley and I (1997) considered the well-known formula for \( \zeta(3) \), used by Apéry in his irrationality proof. Recall that there are no immediately analogous formulae for \( \zeta(5), \zeta(7), \ldots \).

In other words, any relatively prime integers \( p \) and \( q \) such that

\[
\zeta(5) \equiv \frac{p}{q} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^5 \binom{2k}{k}}
\]

have \( q \) astronomically large.

- A less known formula for \( \zeta(5) \) due to Koecher suggested generalizations for \( \zeta(7), \zeta(9), \ldots \). Again the coefficients were obtained by an LLL integer relation algorithm. Bootlegging the earlier pattern kept the search space of manageable size.
For example, and already simpler than Koecher, 
\[ \zeta(7) = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k^7 \binom{2k}{k}} + \frac{25}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k+1} k^{-1}}{k^3 \binom{2k}{k}} \sum_{j=1}^{k-1} \frac{1}{j^4}. \]

We were able – by finding integer relations for \( n = 1, 2, \ldots, 10 \) – to encapsulate the formulae for \( \zeta(4n+3) \) in a single conjectured generating function (ex machina):

\[ \sum_{n=1}^{\infty} \zeta(4n+3) z^{4n} \]
\[ = \sum_{k=1}^{\infty} \frac{1}{k^3 (1 - z^4 / k^4)} \]
\[ = \frac{5}{2} \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^3 \binom{2k}{k}} \frac{1}{(1 - z^4 / k^4)} \prod_{m=1}^{k-1} \frac{1 + 4z^4 / m^4}{1 - z^4 / m^4}. \]
• We proved many reformulations of (4), including a finite sum:* 

\[
\sum_{k=1}^{n} \frac{2n^2}{k^2} \frac{\prod_{i=1}^{n-1} (4k^4 + i^4)}{\prod_{i=1, i\neq k}^{n} (k^4 - i^4)} = \binom{2n}{n}.
\]

◊ This identity† was recently proved by Almkvist and Granville, thus finishing the proof of (4) and giving a rapidly converging series for any \(\zeta(4n + 3)\) where \(n\) is positive integer.

**Question.** What of \(\zeta(4N + 1)\)? There are *too many* identities.

**Coworkers:** Bradley, Almkvist, Fee, Granville

*Found via Gosper’s algorithm after by a mistake in an electronic Petrie dish.

†Erdos, when shown this shortly before his death, rushed off. Twenty minutes later he returned saying he did not know how to prove it but if proven it would have implications for Apéry’s result.
F. From Euler to Zagier

- Very large scale: mixing fields/tool/interfaces etc.

- *Euler sums* or “multiple zeta functions” (MZVs) are a wonderful generalization of the classical $\zeta$. For positive integers $i_1, i_2, \ldots, i_k$

\[(6)\]

$$\zeta(i_1, i_2, \ldots, i_k) := \sum_{n_1>n_2>\ldots>n_k>0} \frac{1}{n_1^{i_1} n_2^{i_2} \cdots n_k^{i_k}}$$

- Note $i_1 > 1$ is necessary and sufficient condition for convergence. Thence we study the mapping

$$\zeta : (\mathbb{N}^+)^k \to \mathbb{R} \cup \{\infty\}.$$  

The integer $k$ is the *depth* of the sum, and $i_1 + i_2 + \cdots + i_k$ is its *weight*.

- Definition (6) clearly extends to alternating sums. MZVs have recently found very interesting interpretations in high energy physics and knot theory, etc.  .
• MZVs satisfy many striking identities, of which \( \zeta(2,1) = \zeta(3) \) is the simplest. (Euler himself found and partially proved theorems on reducibility of depth 2 to depth 1 zetas.)

◊ Our recent work on integral representations of Euler sums led to a fast algorithm* for very high precision evaluations; thus allowing us to thoroughly examine them using integer relation algorithms. This leads to amazing identities and dimensional conjectures†.

• The example we detail here is motivated by the identity conjectured by Zagier and proved by Broadhurst, after extensive empirical work by BBBL:

\[
\zeta(\{3, 1\}_n) = \frac{1}{2n + 1} \zeta(\{2\}_{2n}) \quad (= \frac{2\pi^{4n}}{(4n + 2)!})
\]

where \( \{s\}_n \) is the string \( s \) repeated \( n \) times.

*A H"older convolution at www.cecm.sfu.ca/projects/EZFace/

†Our simplest dimensional conjectures are surely beyond present proof techniques. Does \( \zeta(5), G \in \mathbb{Q}? \).
• In all known “non-decomposable” identities for Euler sums, all $\zeta$-terms have the same weight. This is of great importance for guided integer relation searches—as it dramatically reduces the size of the search space.

• Broadhurst and Lisoněk then used Bailey’s fast implementation of the PSLQ algorithm to search for generalizations of Zagier’s identity.

◊ It soon appeared that the “cycles"

$$Z(m_1, m_2, \ldots, m_{2n+1}) := \zeta([2] m_1, 3, [2] m_2, 1, [2] m_3, 3, \ldots, 1, [2] m_{2n+1}).$$

participate in many such identities. Checking PSLQ input vectors from all $Z$ values of fixed weight ($2K$, say) along with the value $\zeta([2]_K)$ detected many identities, from which general patterns were “obvious”.

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• This led to a conjecture (among many):*

\[
\sum_{i=0}^{2n} Z(C^i S) \equiv \zeta(\{2\}_M + 2n)
\]

for \( S \) a string of \( 2n + 1 \) non-negative integers summing to \( M \), and \( C^i S \) the cyclic shift of \( S \) by \( i \) places.

Zagier’s identity is the case of (7) with entries of \( S \) zero.

• The symmetry in (7) highlighted that Zagier-type identities have serious combinatorial content. For \( M = 0, 1 \) we could to reduce (7) to evaluation of combinatorial sums; and thence to truly combinatorial proofs.†

**Coworkers:** Bailey, D. Borwein, Bradley, Broadhurst, Girgensohn, Lisoněk, Yazdani

*My favourite is

\[
8^n \zeta(\{-2, 1\}_n) \equiv \zeta(\{2, 1\}_n).
\]

Can \( n = 2 \) be proven symbolically?

†For \( M \geq 2 \) we have no proofs, but very strong evidence.
G. From Zagier to Kontsevich?

- The prototype of our hunt is a remarkable relation between Clausen values: \( \text{vol}(6^3_1) = \)

\[
3\text{Cl}_2(\theta_7) - 3\text{Cl}_2(2\theta_7) + \text{Cl}_2(3\theta_7) = \frac{7}{2} \times 
\]

\[
(8) \left\{ \text{Cl}_2 \left( \frac{2\pi}{7} \right) + \text{Cl}_2 \left( \frac{4\pi}{7} \right) - \text{Cl}_2 \left( \frac{6\pi}{7} \right) \right\} 
\]

with

\[
\theta_7 := 2 \arctan \sqrt{7}.
\]

- Here the volume is the hyperbolic volume of the link \((\sigma_1^2\sigma_2^{-1})^2\) and Clausen’s function

\[
\text{Cl}_2(\theta) := \sum_{k=1}^{\infty} \frac{\sin(k\theta)}{k^2}
\]

is an imaginary part, \(\text{Li}_2(\exp(i\theta))\), of the dilogarithm

\[
\text{Li}_2(z) := \sum_{k=1}^{\infty} \frac{z^k}{k^2}.
\]
How this was done?

- We were initially looking for links whose volumes had closed forms. So quadratic orthoschemes were computed in *snappea* and then pieced together with a prodigious quantity of computing in PSLQ + PARI + Maple + Databases.

1. Solved for all 10 possible Schlafli functions with $\tan(\delta)^2 \in \mathbb{Q}$. Noted the first few have only $\pm$ coefficients at division points of the circle. Thence, identified (8) and 9 other quadratic cases as values of Dedekind L-series at 2.

2. Guessed that the field’s discriminant and number of real places were important. Accessed the Bordeaux number fields with $[n-2,1]$, $n = 2, 3, 4, 5, 6, 7$. Computed $\zeta_K(2)$ for the first 200 entries for each.

*www.geom.umn.edu/software/download/snappea.html
3. Accessed all the Hodgson-Weeks census of closed manifolds. The intersection scored 96 ‘hits’ of $\zeta_K(2)$ (onto 175 distinct manifold volumes).

4. Accessed all the fields found by CGHN (Coulson, Goodman, Hodgson and Neumann, 1985) in the census, by polynomial fitting. Computed the signatures and discriminants of each and looked at the overlap with the Bordeaux hits.

5. All of CGHN’s finds in the above Bordeaux range were already in the $\zeta_K$ hitlist. One of those hits wasn’t in the CGHN list: so we has a stone-cold prediction.
• **(Re?)-Conjecture (Borwein-Broadhurst):** Every closed hyperbolic manifold*, \( M \), whose invariant trace field, \( K \), has precisely one complex place has a volume, \( \text{vol}(M) \), satisfying

\[
\frac{12\zeta_K(2)|D|^{3/2}}{(2\pi)^{2n-2}} = q_M \text{vol}(M)
\]

where \( \zeta_K \), \( D \) and \( n \) are the Dedekind zeta function, discriminant and order of \( K \), and \( q_M \) is a (small) rational number.

◊ **Comment:** This has been tested on all the closed manifolds that CGHN related to number fields with one complex place and \(-D \leq 202,734,487 \cdots \) and then some of degree 9 and 11.

In toto, 212 distinct volumes were related to 129 distinct number fields where the last 33 lay outside the chosen Bordeaux ranges.

**Coworkers:** Broadhurst, Broadhurst and Broadhurst

*The manifolds come from Dehn surgery on knots/links.*
The scope of the C3.ca is a seven year plan to build computational infrastructure on a scale that is globally competitive, and that supports globally competitive research and development. The plan will have a dramatic impact on Canada’s ability to develop a knowledge based economy. It will attract highly skilled people to new jobs in key application areas in the business, research, health, education and telecommunications sectors. It will provide the tools and opportunity to enhance their knowledge and experience and retain this resource within the country.

- 25% of Memorial University’s large Dec Alpha was used for Euler sum research in the past 18 months.