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π AT THE LIMITS OF COMPUTATION

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Dedicated to late Professor Dario Castellanos (1937-1995) *of Facultad de Ingeniería, Universidad de Carabobo, Valencia, Venezuela.*

Abstract. Before 1976, all record-broken computation for the digits of π completely depended on arctangent-type identities; of them the most celebrated is John Machin's identity $\frac{\pi}{4} = 4\tan^{-1}(\frac{1}{5}) - \tan^{-1}(\frac{1}{239})$, discovered in 1706. But, in 1976, Eugene Salamin moved in a powerful heavy artillery. The method is an adaptation of an algorithm discovered by Gauss for the evaluation of elliptic integrals. Then, a new era comes. In 1983, Y. Kanada, Y. Tanura, S. Yoshino and Y. Ushiro used Gauss-Legendre-Brent-Salamin algorithm to calculate π to 2^{24} (16,777,216) decimal places on a HITAC M-280H supercomputer and used an FFT-based fast multiplication. In this article, we present an easy-to-understand explanation of this amazing method.

In 1976, Eugene Salamin of Stanford, California, published in *Mathematics of Computation* an ingenious, quadratically converging algorithm for the calculation of π [10]. Quadratically converging means the number of significant figures doubles after each step. The method is an adaptation of an algorithm discovered by Gauss for the evaluation of elliptic integrals.

The complete elliptic integrals of the first and second kinds are defined by

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{dt}{\sqrt{(1-k^2\sin^2 t)}} \tag{1}$$

and

$$E(k) = \int_0^{\frac{\pi}{2}} \sqrt{(1-k^2\sin^2 t)}dt.$$

It $k^2 + k'^2 = 1$, then $K(k') = K'(k)$, and $E(k') = E'(k)$ are also elliptic integrals, and they satisfy Legendre's relation:

$$K(k)E'(k) + K'(k)E(k) - K(k)K'(k) = \frac{\pi}{2}. \tag{2}$$

If $\{a_n\}$ is a convergent sequence with limit L, and if there exists a constant C, such that

$$|a_n - L| \leq C|a_n - L|^2$$

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for all n, then the sequence $\{a_n\}$ is said to converge quadratically to L.

Consider a triple of positive nubmers (a_0, b_0, c_0) satisfying $a_0^2 = b_0^2 + c_0^2$. We proceed to determine number triples (a_1, b_1, c_1), $(a_2, b_2, c_2), \ldots, (a_N, b_N, c_N)$ according to the following scheme of arithmetic-geometric means:

$$\begin{array}{ccc} a_0 & b_0 & c_0 \\ a_1 = \frac{1}{2}(a_0 + b_0) & b_1 = \sqrt{(a_0 b_0)} & c_1 = \frac{1}{2}(a_0 - b_0) \\ a_2 = \frac{1}{2}(a_1 + b_1) & b_2 = \sqrt{(a_1 b_1)} & c_2 = \frac{1}{2}(a_1 - b_1) \\ \cdots & \cdots & \cdots \\ a_N = \frac{1}{2}(a_{N-1} + b_{N-1}) & b_N = \sqrt{(a_{N-1} b_{N-1})} & c_N = \frac{1}{2}(a_{N-1} - b_{N-1}) \end{array}$$

As a consequence of the arithmetic-geometric mean inequality one has $a_n \geq a_{n+1} \geq b_{n+1} \geq b_n$ for all n. It follows that $\{a_n\}$ and $\{b_n\}$ converge to a common limit, usually denoted by $agm(a_0, b_0)$.

Because of the definition of the c's above one easily obtains

$$c_{n+1} = \frac{1}{2}(a_n - b_n) = \frac{c_n^2}{4a_{n+1}} \leq \frac{c_n^2}{4agm(a_0, b_0)},$$

and we see that the sequence $\{c_n\}$ converges quadratically to zero.

In calculations one stops at the Nth step, when $a_N = b_N$, i.e., when $c_N = 0$ to the desired degree of accuracy.

The substitution $k^2 \to \frac{a^2 - b^2}{a^2}$, $a > b$ shows that equation (1) can, apart from a constant factor, be put into the form

$$I(a, b) = \int_0^{\frac{\pi}{2}} \frac{dt}{\sqrt{(a^2 \cos^2 t + b^2 \sin^2 t)}}. \tag{3}$$

The substitution $u = b \tan t$ transforms (3) into the integral

$$I(a, b) = \frac{1}{2} \int_{-\infty}^{0} \frac{du}{\sqrt{(a^2 + u^2)(b^2 + u^2)}}.$$

The substitution $v = \frac{1}{2}(u - \frac{ab}{u})$ and some straightforward but elaborate work shows that

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

This remarkable result, due to Gauss [6], shows that $I(a_n, b_n)$ is independent of n and that, interchanging the limit and the integral,

$$I(a_0, b_0) = \lim_{n \to \infty} I(a_n, b_n) = I(agm(a_0, b_0), agm(a_0, b_0)).$$

The last integral is elementary and we have

$$I(a_0, b_0) = \frac{\pi}{2agm(a_0, b_0)}.$$

With $a_0 = 1$, $b_0 = \cos\alpha$, $c_0 = \sin\alpha$, and $K(\alpha)$ for $K(\sin\alpha)$ one has, to the desired degree of accuracy,

$$K(\alpha) = \frac{\pi}{2a_N}, \tag{4}$$

$$\frac{K(\alpha) - E(\alpha)}{K(\alpha)} = \frac{1}{2}[c_0^2 + 2c_1^2 + 2^2c_2^2 + \cdots + 2^N c_N^2]. \tag{5}$$

Also with $a_0' = 1$, $b_0' = \sin\alpha$, $c_0' = \cos\alpha$,

$$K'(\alpha) = \frac{\pi}{2a_N'}, \tag{6}$$

$$\frac{K'(\alpha) - E'(\alpha)}{K(\alpha)} = \frac{1}{2}[c_0'^2 + 2c_1'^2 + 2^2c_2'^2 + \cdots + 2^N c_N'^2]. \tag{7}$$

Salamin's idea was to evaluate each of the elliptic integrals in Legendre's relation (2) by Gauss's arithmetic-geometric mean, equations (4) to (7), and then solve for π!

With k and k' as defined before, i.e., $k^2 + k'^2 = 1$, then

$$\pi = \frac{4agm(1,k)agm(1,k')}{1 - \sum_{j=1}^{\infty} 2^j(c_j^2 + c_j'^2)}. \tag{8}$$

With the symmetric choice $k = k' = \frac{1}{\sqrt{2}}$, (8) becomes

$$\pi = \frac{4\left(agm\left(1, \frac{1}{\sqrt{2}}\right)\right)^2}{1 - \sum_{j=1}^{\infty} 2^{j+1}c_j^2}.$$

A number of significant improvements on Salamin's original approcah have been achieved by the Canadian brothers Jonathan M. Borwein and Peter B. Borwein. Their results can be summarized as follows [1, 2, 3, 4]:

Algorithm 1.

Let $\alpha_0 = \dfrac{1}{2}$, $y_0 = \dfrac{1}{\sqrt{2}}$, $y_{n+1} = \dfrac{1 - \sqrt{1 - y_n^2}}{1 + \sqrt{1 - y_n^2}}$, and $\alpha_{n+1} = (1 + y_{n+1})^2\alpha_n - 2^{n+1}y_{n+1}$.

Then $0 < \alpha_n - \dfrac{1}{\pi} \leq \dfrac{16 \cdot 2^n}{e^{2^n\pi}}$, i.e., α_n converges quadratically to $\dfrac{1}{\pi}$.

Algorithm 2.

Let $\alpha_0 = 6 - 4\sqrt{2}$, $y_0 = \sqrt{2} - 1$, $y_{n+1} = \dfrac{1 - \sqrt[4]{1 - y_n^4}}{1 + \sqrt[4]{1 - y_n^4}}$, and $\alpha_{n+1} = (1+y_{n+1})^4\alpha_n - 2^{2n+3}y_{n+1}(1+y_{n+1}+y_{n+1}^2)$.

Then $0 < \alpha_n - \dfrac{1}{\pi} \le \dfrac{16\cdot 4^n}{e^{2\cdot 4^n\pi}}$, i.e., α_n converges quartically to $\dfrac{1}{\pi}$.

Algorithm 3.

Let $s_0 = 5(\sqrt{5}-2)$, $\alpha_0 = \dfrac{1}{2}$, and $s_{n+1} = \dfrac{25}{\left(z+\frac{x}{z}+1\right)^2 s_n}$,

where $x = \dfrac{5}{s_n} - 1$, $y = (x-1)^2 + 7$, $z = \sqrt[5]{\left[\dfrac{1}{2}x\left(y+\sqrt{y^2-4x^3}\right)\right]}$.

Let $\alpha_{n+1} = s_n^2\alpha_n - 5^n\left[\dfrac{s_n^2-5}{2} + \sqrt{s_n(s_n^2-2s_n+5)}\right]$.

Then $0 < \alpha_n - \frac{1}{\pi} \le \dfrac{16\cdot 5^n}{e^{5^n\pi}}$, i.e., α_n converges quintically to $\dfrac{1}{\pi}$.

Note that, for four iterations, algorithm 1 gives 19 digits of π, algorithm 2 gives 694 digits of π, algorithm 3 gives 848 digits of π.

The simplicity and power of algorithm 2 has led the Borweins to term it "the most efifcient algorithm currently known for the extended precision calculation of pi." Thirteen iterations of it yield in excess of one billion decimal places of π!

The underlying mathematics behind these algorithms is far from simple. They all rely heavily on some pioneering work of Ramanujan on the solution of modular equations by methods which have yet to be fully understood. Mathematicians have verified the correctness of some of Ramanujan's results in this area with recourse to advanced techniques of group theory or even with the use of sophisticated algebraic manipulation packages, such as MACSYMA, which were clearly unavailable to him. The natural and evidently ingenious methods Ramanujan possessed remain still to be rediscovered.

Modular equations, Jacobian elliptic functions, elliptic integrals and the arithmetic-geometric mean are all intimately connected. These connections are explained in considerable detailed in Borwein and Borwein's book *Pi and the AGM – A Study in Analytic Number Theory and Computational Complexity*, Wiley, N. Y., 1987. The reader is warned, though, that this is not a book for beginners. A considerable familiarity with the theory of analytic functions of a complex variable is assumed.

If a_n and b_n designate the reciprocals of the perimeters of the circumscribed and inscribed regular $6\cdot 2^n$-gons about a circle of diameter 1, then $a_0 = \frac{1}{2\sqrt{3}}$, $b_0 = \frac{1}{3}$ and the Archimedean iteration may be put in the form

$$a_{n+1} = \frac{1}{2}(a_n+b_n) \quad \text{and} \quad b_{n+1} = \sqrt{(a_{n+1}b_n)}. \tag{9}$$

This fact was first noticed by Johann Friedrich Pfaff (1765-1825) in 1800.

Equations (9) are remarkably similar to the arithmetic-geometric mean iteration

$$a_{n+1} = \frac{1}{2}(a_n+b_n), \quad b_{n+1} = \sqrt{(a_nb_n)}. \tag{10}$$

Nonetheless, (10) is, as we have seen, quadratically convergent while (9) gives linear convergence.
The arithmetic-geometric mean is homogeneous, i.e.,

$$agm(\lambda a, \lambda b) = \lambda agm(a, b). \tag{11}$$

There is no restriction, then, in setting $a = 1$.

The arithmetic-geometric mean satisfies the equation

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

or, in view of (11), the equation

$$agm(1, b) = \frac{1+b}{2} agm\left(1, \frac{2\sqrt{b}}{1+b}\right). \tag{12}$$

This shows that solving (12) is equivalent to finding a function $f(x)$ that satisfies the equation

$$f(x) = \frac{1+x}{2} f\left(\frac{2\sqrt{x}}{1+x}\right).$$

Since the complete elliptic integral of the first kind is related to the arithmetic-geometric mean through equation (4), we see that $K(x)$ satisfies the functional equation

$$K(x) = \frac{1}{1+x} K\left(\frac{2\sqrt{x}}{1+x}\right). \tag{13}$$

If we assume [8] that, apart from the multiplicative constant $\frac{\pi}{2}$, $K(x)$ admits the series expansion $K(x) = 1 + k_1x^2 + k_2x^4 + \cdots$, then (13) gives

$$K(x) = \frac{1}{1+x} + \frac{4k_1x}{(1+x)^3} + \frac{16k_2x^2}{(1+x)^5} + \cdots$$

The relation between the coefficients can now be obtained by means of the array

$$\begin{array}{ccccc}
1 & -1 & 1 & -1 & 1 \\
 & 4k_1 & -4k_1 \cdot 3 & 4k_1 \cdot 6 & -4k_1 \cdot 10 \\
 & & 16k_2 & -16k_2 \cdot 5 & 16k_2 \cdot 15 \\
 & & & 64k_3 & -64k_3 \cdot 7 \\
 & & & & 256k_4 \\
\hline
1 & 0 & k_1 & 0 & k_2
\end{array}$$

They give $K(x) = 1 + (\frac{1}{2})^2x^2 + (\frac{1\cdot 3}{2\cdot 4})^2x^4 + (\frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6})^2x^6 \cdots$, which is recognized as Gauss's hypergeometric function:

$$K(k) = \int_0^{\frac{\pi}{2}} \frac{dt}{\sqrt{(1 - k^2 \sin^2 t)}} = \frac{\pi}{2^2} F_1\left(\frac{1}{2}, \frac{1}{2}; 1; k^2\right), \tag{14}$$

and provides a link between the arithmetic-geometric mean and the hypergeometric function. (14) may be obtained directly by expanding the radical in the integrand by Newton's binomial theorem and integrating term by term [9].

In 1989, Gregory V. and David V. Chudnovsky of Columbia University carried the tail of π to 1,011,196,691 decimal places. They used a CRAY 2 at the Minnesota Supercomputer Center and an IBM 3090 at the Thomas J. Watson Research Center in Yorktown Heights, New York [5]. The programming was done in ordinary FORTRAN, and their calculations were made in batch mode, in a environment shared by many users.

Their algorithm is based on a series of the same type as Ramanujan's

$$\frac{1}{\pi} = \frac{\sqrt{8}}{9801} \sum_{n=0}^{\infty} \frac{(4n)!}{(n!)^4} \frac{(1,103 + 26,390n)}{396^{4n}},$$

and it is given by:

$$\frac{1}{\pi} = \frac{1}{426,880\sqrt{10,005}} \sum_{n=0}^{\infty} \frac{(-1)^n (6n)!}{(n!)^3 (3n)!} \frac{(13,591,409 + 545,140,134n)}{640,320^{3n}}. \tag{15}$$

For purposes of calculation they put series (15) in the form

$$\frac{426,880\sqrt{10,005}}{\pi} = b - \frac{1}{1}\frac{3}{1}\frac{5}{1}e\left(a + b - \frac{7}{2}\frac{9}{2}\frac{11}{2}e\left(2a + b - \frac{13}{3}\frac{15}{3}\frac{17}{3}e\left(3a + b - \cdots\right.\right.\right. \tag{16}$$

with $a = 545,140,134$, $b = 13,591,409$, and $e = (320,160)^{-3}$.

Summing this series to N terms determines π to $14.18N$ decimal places. This series is related to the quadratic field $\boldsymbol{Q}(\sqrt{-163})$, which is the largest-one-class imaginary quadratic field, and it is the one with the most rapidly converging right-hand side in which every summand is a rational number. In other words, of all the series which converge to $\frac{1}{\pi}$, series (16) is the most rapidly converging one all of whose summands are rational numbers.

This rationality became a crucial issue for the Chudnovsky brothers for they regard the series as the expansion of a number in radix $640,320^{-3}$. The coefficients in that base are all integers.

Operating in the integers modulo p for a prime p that does not divide 640,320, the Chudnovsky brothers made use of the relationship:

$$\sum_{n=0}^{N} \frac{(-1)^n (6n)!}{(n!)^3 (3n)!} \frac{(13,591,409 + 545,140,134n)}{640,320^{3n}} \equiv 0 (\mathrm{mod} p)$$

which holds for primes p in the range from N to $6N$.

These congruences, together with other specialized congruences, known as p-adic relations, permitted them to check the correctness of their calculation as they proceeded. These checks assured them that the probability of an uncorrected error at any step was less than 10^{-290}.

On 20th September, 1999, Yasumasa Kanada and Daisuke Takahashi, with a HITACHI SR8000 at the University of Tokyo, using Gauss-Legendre-Brent-Salamin algorithm as the main program and Borwein's 4-th order convergent algorithm as the verification program, arrived to the incredible boundary of 206,158,430,000 decimal places. The elapsed time was 37 hours and 21 minutes.

There exists another extraordinary series of Ramanujan,

$$\frac{1}{\pi} = \sum_{n=0}^{\infty} \binom{2n}{n}^3 \frac{42n+5}{2^{12n+4}}.$$

The numerators of this series grow like 2^{6n}, and the denominators are exactly $16 \cdot 2^{12n}$. This fact can be used to calculate the second block of n binary digit of π without calculating the first n binary digit. This interesting observation, due to Holloway [4], results, unfortunately, in no reduction in complexity.

Philip J. Davis, of Brown University, mentioned the following anecdote in private communication to Darío Castellanos: Davis asked Daniel Shanks of the University of Maryland, who, it will be remembered, together with John W. Wrench, Jr., did the first calculation of π with 100,000 places in 1961, the question of how many operations were needed to calculate π to n places? On the basis of his answer, Shanks predicted that mankind would never see one billion digits of π. We have seen this prediction fall with the Chinese proverb to the effect that *it is silly to make predictions, especially with regard to the future.*

Peter B. Borwein has now put forward the conjecture [7] that mankind will never know the $10^{1000}th$ digit of π. The only way to know that digit – he reasons – would be to compute all the digits that come before. And since, all told, the universe does not contain that many electrons, the project – he says – seems unlikely to succeed.

Will Borwein's mark be toppled too?

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