On the Zeros of the Riemann Zeta Function in the Critical Strip. II

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Abstract. We describe extensive computations which show that Riemann's zeta function $\zeta(s)$ has exactly 200,000,001 zeros of the form $\sigma + it$ in the region $0 < t < 81,702,130.19$; all these zeros are simple and lie on the line $\sigma = \frac{1}{2}$. (This extends a similar result for the first 81,000,001 zeros, established by Brent in *Math. Comp.*, v. 33, 1979, pp. 1361–1372.) Counts of the numbers of Gram blocks of various types and the failures of "Rosser's rule" are given.

1. Introduction. Riemann's zeta function is the meromorphic function ζ: $\mathbf{C} \setminus \{1\} \to \mathbf{C}$, which, for $\mathrm{Re}(s) > 1$, may be represented explicitly by

$$\zeta(s) = \sum_{n=1}^{\infty} n^{-s} \qquad (s = \sigma + it).$$

It is well known (see Titchmarsh [16, Chapters II and X]) that

$$\xi(s) := \tfrac{1}{2}s(s - 1)\pi^{-s/2}\Gamma(s/2)\zeta(s)$$

is an entire function of order 1, satisfying the functional equation $\xi(s) = \xi(1 - s)$, so that

$$\Xi(z) := \xi\left(\tfrac{1}{2} + iz\right) \qquad (z \in \mathbf{C}),$$

being an even entire function of order 1, has an infinity of zeros. The Riemann Hypothesis is the statement that all zeros of $\Xi(z)$ are real, or, equivalently, that all nonreal zeros of $\zeta(s)$ lie on the "critical" line $\sigma = \frac{1}{2}$. Since $\zeta(\bar{s}) = \overline{\zeta(s)}$, we may restrict ourselves to the half plane $t > 0$. To this day, Riemann's Hypothesis has neither been proved nor disproved.

Numerical investigations related to this unsolved problem were initiated by Riemann himself and later on continued more systematically by the writers listed below (including their progress).

Investigator	Year	The first n complex zeros of $\zeta(s)$ are simple and lie on $\sigma = \frac{1}{2}$
Gram [6]	1903	$n = 15$
Backlund [1]	1914	$n = 79$
Hutchinson [7]	1925	$n = 138$
Titchmarsh [15]	1935/6	$n = 1,041$

Those listed above utilized the Euler-Maclaurin summation formula and performed their computations by hand or desk calculator, whereas those listed below applied the Riemann-Siegel formula in conjunction with electronic computing devices.

Lehmer [10], [11]	1956	$n = 25,000$
Meller [13]	1958	$n = 35,337$
Lehman [9]	1966	$n = 250,000$
Rosser, Yohe & Schoenfeld [14]	1968	$n = 3,500,000$
Brent [2]	1979	$n = 81,000,001$

An excellent explanatory account of most of these computations may be found in Edwards [4].

In this paper, which should be considered as a continuation of Brent [2]*, we report on extensive computations by which the first named author has extended his former result to $n = 156,800,001$ and by which the remaining three authors (L R & W, for short) have extended this bound to $n = 200,000,001$. Details of the last result, together with a full program listing, are given in van de Lune, te Riele and Winter [12]. Independently of Brent, L R & W have also checked the range $[g_{81,000,000}, g_{120,000,000})$.

In practice, the numerical verification of the Riemann hypothesis in a given range consists of separating the zeros of the well-known real function $Z(t)$ (see formula (2.6) of Brent [2]), or, equivalently, of finding sufficiently many sign changes of $Z(t)$. Our programs (aiming at a fast separation of these zeros) are based, essentially, on the modification of Lehmer's [11] method introduced by Rosser et al. [14]. L R & W have developed a more efficient strategy of searching for sign changes of $Z(t)$ in Gram blocks of length $L \geqslant 2$. Brent's average number of Z-evaluations, needed to separate a zero from its predecessor, amounts to about 1.41 (compare Brent [2]), whereas L R & W have brought this figure down to about 1.21. It may be noted here that in the most recent version of the program of L R & W this figure has been reduced further to about 1.185. From the statistics in Section 4, it follows that in the range $[g_{156,800,000}, g_{200,000,000})$ this average number of Z-evaluations could not have been reduced below 1.135 by any program which evaluated $Z(t)$ at all Gram points. We also note that about 98 percent of the running time of the L R & W-program was spent on evaluating $Z(t)$. This program was executed on a CDC CYBER 175 computer and ran about ten times as fast as the UNIVAC 1100/42 program of Brent. This is roughly what could be expected, given the relative speeds of the different machines.

2. The Strategy for Finding the Required Number of Sign Changes of $Z(t)$ in a Gram Block of Length $L \geqslant 2$. The strategy of Brent for finding the required number of sign changes of $Z(t)$ is exactly as described in Section 4 of Brent [2]. L R & W refined this strategy in order to reduce the number of Z-evaluations as much as they could. This will be described here in some detail.

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* We take the opportunity to make the following corrections in Brent [2]: on p. 1361, line 9 ↑ , replace "$H(10)$" by "$H(15)$"; on p. 1362, Eq. (2.3), replace "B_{2k}" by "$| B_{2k} |$".

In order to reduce the number of Z-evaluations as much as possible, we first observe that after having determined a Gram block B_j of length $L \geqslant 2$, we already have implicitly detected $L - 2$ sign changes of $Z(t)$. Hence, the problem reduces to finding the "missing two" sign changes. Next we observe that these missing two (if existing) must both lie in one and the same Gram interval of the block B_j. Some preliminary experiments with the L R & W-program revealed that in the majority of cases the missing two are situated in one of the *outer* Gram intervals of B_j. Therefore, we first search in (g_j, g_{j+1}) or (g_{j+L-1}, g_{j+L}) according to which of abs($Z(g_j) + Z(g_{j+1})$) and abs($Z(g_{j+L-1}) + Z(g_{j+L})$) is the smallest. In the selected interval an efficient parabolic interpolation search routine is invoked. (Here is the main improvement over Brent's method, which used random search rather than parabolic interpolation.) If this routine terminates without having found the missing two sign changes, the other outer Gram interval of the block is treated in the same manner. In case the missing two are still not found, another search routine is called, depending on the length L of the block $B_j = [g_j, g_{j+L})$.

If $L = 2$, the interval (g_j, g_{j+2}) is scanned again, and if $L > 2$, we continue to search in the interval (g_{j+1}, g_{j+L-1}). In both cases, the search is performed by means of a refinement of a search routine described by Lehman [9]. For more details we refer the reader to the source text of the L R & W-program in [12].

If at some instant one of the search routines has detected the missing two, a new Gram block is set up, and we continue as described above. In the opposite case the program prints a message and a "plot" of $Z(t)$ corresponding to the whole Gram block under investigation and proceeds by pretending (!) that the missing two were found indeed. These plots of $Z(t)$ were inspected afterwards (if necessary) "by hand". So far, the missing two were always easily found either in the Gram block under consideration or in an adjacent Gram block; compare Brent [2, Section 4].

After having covered the range $[g_{156,800,000}, g_{200,000,000})$, we ran the computation a little further and found 4 Gram blocks in $[g_{200,000,000}, g_{200,000,004})$, all of them satisfying Rosser's rule. By applying Theorem 3.2 of Brent [2], we completed the proof of our claim that the first $n = 200,000,001$ zeros of $\zeta(s)$ are simple and lie on $\sigma = \frac{1}{2}$.

We (L R & W) intend to extend our computations in the near future.

3. Computation of $Z(t)$ and Error Analysis. In principle, Brent's and L R & W's methods of computing $Z(t)$ and error analysis are exactly as described in Section 5 of Brent [2]. We shall only mention here the differences between L R & W's computations and error analysis and Brent's. Details are given in [12].

The L R & W-computations were carried out on a CDC CYBER 175 computer having a 60-bit word, and single-precision and double-precision floating point arithmetic using 48- and 96-bit binary fractions, respectively. The function $Z(t)$ was computed (in both methods A and B) using the Riemann-Siegel formula with *two* terms in its asymptotic expansion. Gabcke's error bound (see [5]) $|R_1(t)| <$ $0.053t^{-5/4}$, for $t \geqslant 200$, was used. The same bound is also given as a special case of more general bounds in Brent and Schoenfeld [3]. For method A, a precomputed table of 8194 cosine-values, and a precomputed table of 8193 corresponding *differences* of cosine-values, was used in the linear interpolation formula for the cosine-approximation. The main loop in method A was programmed in machine

language (COMPASS), and one cycle of this loop executed in about 2.1 μsec. The error analysis, accounting for *all* possible errors in the machine computation of $Z(t)$, was carried out for any t in the interval $(3.5 \times 10^7, 3.72 \times 10^8)$. This interval covers the range of zero #81,000,000 till zero #1,000,000,000 of $\zeta(s)$ in the critical strip, which L R & W originally planned to investigate. The following bounds for the error in the computed value $\tilde{Z}(t)$ of $Z(t)$ were derived:

$$|\tilde{Z}(t) - Z(t)| \leq \begin{cases} 3 \times 10^{-7}\tau^{1/4} & \text{for method A,}** \\ (5.4 \times 10^{-3}\tau^{-3/2} + 3.1 \times 10^{-16} + 4.1 \times 10^{-24}\tau^{-1/2} \\ \qquad + 5 \times 10^{-26}\tau \ln(\tau))\tau^{1/4} & \text{for method B,} \end{cases}$$

for any t ($= 2\pi\tau$) in the interval $(3.5 \times 10^7, 3.72 \times 10^8)$. In this interval, a safe upper bound for the error is 2.7×10^{-5}, respectively 2.0×10^{-11}. In the L R & W-program, the extremely conservative *fixed* bounds 10^{-4} (and sometimes even 2×10^{-4}) respectively 2.5×10^{-6} were used. Nevertheless, until now not a single t was met for which method B could not determine the sign of $Z(t)$ rigorously.

4. Statistics. The L R & W-program was organized in such a way that in case the value of $Z(t)$, obtained with method A, was too small for a rigorous sign determination, a few small shifts of the argument were tried before method B was invoked. Therefore, the L R & W-program uses, in relatively few cases, an approximation to the Gram point g_j instead of g_j itself. (In a run of 2,500,000 zeros, with error bound 10^{-4} for method A, the *total* number of shifts was always less than 370. Most of them were made when separating the zeros *inside* the Gram blocks. Only a few of them were made in Gram points. Also see the text introducing Table 3.) Consequently, the statistics found by L R & W cannot, strictly speaking, be accumulated to those found by Brent. Nevertheless, just for convenience, we have put together all results. This should be kept in mind when reading the tables.

In Table 1 we present a list of 104 exceptions to Rosser's rule up to $g_{200,000,000}$ found by Brent and L R & W, including the 15 exceptions up to $g_{75,000,000}$ from [2], for completeness. Moreover, the types are given in parentheses, followed by the local extreme values of $S(t)$ near B_n. It is possible that for $n \geq 156,800,000$ the L R & W-program has not detected *all* exceptions to Rosser's rule, due to possible shifts in Gram points. For instance, an exception of type 2 (see Table 2) may have been detected as a Gram block of length 3 with "2 1 0" zero-pattern. It may be noted, however, that in the range $[g_{81,000,000}, g_{120,000,000})$ L R & W have found exactly the same exceptions to Rosser's rule as Brent.

In addition to the types 1, 2, and 3 introduced by Brent [2], we have defined the types 4, 5, and 6, the meaning of which should be clear from Table 2. This table also gives the frequencies of the occurrences of the various types in $[g_{-1}, g_{200,000,000})$. Note that an exception of type 4 has not yet been found, so that at the time of writing we still know only one Gram interval with four zeros, viz. $G_{61,331,768}$, found by Brent [2].

** In [12] a four-term bound was given for method A. A closer look at the error analysis led us to the simpler bound given here.

TABLE 1
(extension of Table 3 of Brent [2])

104 *exceptions to Rosser's rule up to* $g_{200,000,000}$

Notation: n (type) extreme $S(t)$ where n is the index
of the Gram block B_n containing no zeros.

13,999,525(1) -2.0041	100,788,444(1) -2.0230	146,130,246(2) 2.0005	173,737,614(2) 2.0221
30,783,329(1) -2.0026	106,236,172(1) -2.0184	147,059,770(1) -2.0498	174,102,513(1) -2.0180
30,930,927(2) 2.0506	106,941,328(2) 2.1559	147,896,100(2) 2.0391	174,284,990(1) -2.0181
37,592,215(1) -2.0764	107,287,955(1) -2.0786	151,097,113(1) -2.0043	174,500,513(1) -2.0125
40,870,156(1) -2.0038	107,532,017(2) 2.0728	152,539,438(1) -2.0026	175,710,609(1) -2.0193
43,628,107(1) -2.0242	110,571,044(1) -2.0458	152,863,169(2) 2.0459	176,870,844(2) 2.0125
46,082,042(1) -2.0311	111,885,254(2) 2.0247	153,522,727(2) 2.0027	177,332,733(2) 2.0146
46,875,667(1) -2.0046	113,239,783(1) -2.0306	155,171,525(2) 2.0437	177,902,862(2) 2.0223
49,624,541(2) 2.0018	120,159,903(1) -2.0589	155,366,607(1) -2.0277	179,979,095(1) -2.0182
50,799,238(1) -2.0288	121,424,392(2) 2.0515	157,260,687(2) 2.0363	181,233,727(2) 2.1018
55,221,454(2) 2.0242	121,692,932(2) 2.0616	157,269,224(1) -2.0329	181,625,435(1) -2.0401
56,948,780(2) 2.0177	121,934,171(2) 2.1719	157,755,123(1) -2.0205	182,105,257(6) 2.0084
60,515,663(1) -2.0081	122,612,849(2) 2.0072	158,298,485(2) 2.0273	182,223,560(2) 2.0156
61,331,766(3) -2.0543	126,116,567(1) -2.0106	160,369,051(2) 2.0071	191,116,405(2) 2.0195
69,784,844(2) 2.0637	127,936,513(2) -2.1105	162,962,787(1) -2.0115	191,165,600(2) 2.0283
75,052,114(1) -2.0045	128,710,278(2) 2.0444	163,724,709(1) -2.0163	191,297,535(5) -2.1490
79,545,241(2) 2.0113	129,398,903(2) 2.0431	164,198,114(2) 2.0235	192,485,616(1) -2.0416
79,652,248(2) 2.0066	130,461,097(2) 2.0963	164,689,301(1) -2.1579	193,264,636(6) 2.0055
83,088,043(1) -2.1328	131,331,948(2) 2.0047	164,880,229(2) 2.0308	194,696,968(1) -2.0664
83,689,523(2) 2.0775	137,334,072(2) 2.0239	166,201,932(1) -2.0024	195,876,805(1) -2.0143
85,348,958(1) -2.0095	137,832,603(1) -2.0134	168,573,836(1) -2.0159	195,916,549(2) 2.0546
86,513,820(1) -2.0154	138,799,472(2) 2.0135	169,750,763(1) -2.1036	196,395,161(2) 2.0326
87,947,597(2) 2.0523	139,027,791(1) -2.0031	170,375,507(1) -2.0009	196,676,303(1) -2.0135
88,600,095(1) -2.1394	141,617,806(1) -2.1253	170,704,880(2) 2.0249	197,889,883(2) 2.0034
93,681,183(1) -2.0165	144,454,931(1) -2.0380	172,000,993(2) 2.0608	198,014,122(1) -2.0333
100,316,552(2) 2.0233	145,402,380(2) 2.0012	173,289,941(1) -2.0378	199,235,289(1) -2.0205

TABLE 2
*Various types of exceptions to Rosser's rule and their
frequencies in* $[g_{-1}, g_{200,000,000})$.

g_{n-2}	g_{n-1}	g_n	g_{n+1}	g_{n+2}	g_{n+3}	g_{n+4}	type	frequency
		0	0	3			1	53
	3	0	0				2	47
		0	0	4	0		3	1
0	4	0	0				4	0
		0	0	2	2		5	1
2	2	0	0				6	2

Gram block of length 2 without any zeros

Very recently, Karkoschka and Werner [8] have developed a method for detecting exceptions to Rosser's rule with relatively small computational effort, i.e., by searching in certain selected small ranges of a given t-interval. A comparison of their results with Table 1 shows the power of their method: in $[g_{3,500,000}, g_{50,000,000})$ they found all 9 exceptions to Rosser's rule, and in $[g_{100,000,000}, g_{120,000,000})$ they found 6 of the 9 exceptions.

Table 3 is a continuation of Table 1 of Brent [2]. Six Gram blocks of length 8 were found. The average block length up to $n = 200,000,000$ is 1.1951. We have compared the results of L R & W with those of Brent in the range $[g_{110,000,000}, g_{120,000,002})$. The observed differences were extremely small. Brent's program counted 7,011,482 Gram blocks of length 1, 1,055,511 of length 2 and 230,234 of length 3. The corresponding figures obtained by L R & W were 7,011,494, 1,055,508 and 230,232, respectively. The numbers of Gram blocks of length ≥ 4 were the same for both programs.

TABLE 3

(continuation of Table 1 of Brent [2])

Number of Gram blocks of given length

n	J(1,n)	J(2,n)	J(3,n)	J(4,n)	J(5,n)	J(6,n)	J(7,n)	J(8,n)
80,000,000	56,942,025	8,386,072	1,714,271	260,637	18,807	1,033	34	
90,000,000	63,977,026	9,439,917	1,941,455	299,932	22,257	1,240	46	
100,000,000	71,004,697	10,493,487	2,169,610	340,360	25,813	1,436	54	
110,000,000	78,023,506	11,547,936	2,399,154	381,216	29,601	1,644	61	
120,000,000	85,034,988	12,603,447	2,629,388	422,721	33,500	1,841	74	1
130,000,000	92,041,326	13,659,023	2,860,087	464,955	37,495	2,070	92	1
140,000,000	99,041,526	14,713,754	3,092,451	507,686	41,631	2,332	102	1
150,000,000	106,038,874	15,768,532	3,325,400	550,630	45,795	2,591	114	3
156,800,000	110,793,769	16,486,479	3,484,026	579,999	48,731	2,780	120	3
200,000,000	140,956,084	21,047,520	4,497,856	771,607	68,631	4,031	213	6

TABLE 4

(continuation of Table 2 of Brent [2])

Number of Gram intervals containing exactly m zeros

n	m = 0	m = 1	m = 2	m = 3	m = 4
80,000,000	10,513,316	59,105,832	10,248,390	132,461	1
90,000,000	11,854,362	66,440,792	11,555,331	149,514	1
100,000,000	13,197,331	73,771,910	12,864,188	166,570	1
110,000,000	14,543,760	81,096,629	14,175,463	184,147	1
120,000,000	15,892,224	88,416,806	15,489,718	201,251	1
130,000,000	17,242,449	95,733,829	16,804,996	218,725	1
140,000,000	18,594,089	103,047,955	18,121,824	236,131	1
150,000,000	19,946,624	110,360,313	19,439,504	253,558	1
156,800,000	20,867,682	115,330,181	20,336,593	265,543	1
200,000,000	26,731,720	146,878,417	26,048,007	341,855	1

Table 4 is a continuation of Table 2 of Brent [2]. The percentages of the numbers of Gram intervals up to $n = 200{,}000{,}000$ containing exactly m zeros are 13.4, 73.4, 13.0, and 0.2 for $m = 0$, 1, 2, and 3, respectively. No new Gram intervals with exactly four zeros were found.

Table 5 continues Table 4 of Brent [2]. As yet, no Gram block of type $(7, 1)$ was found. Due to the shifts, we may have missed earlier occurrences of blocks of types $(7, 7)$, $(8, 3)$ and $(8, 7)$, although we consider this unlikely.

TABLE 5

(continuation of Table 4 of Brent [2])

First occurrences of Gram blocks of various types

j	k	n
7	7	195,610,937 (L R & W)
8	2	112,154,948 (BRENT)
8	3	175,330,804 (L R & W)
8	6	145,659,810 (BRENT)
8	7	165,152,519 (L R & W)

TABLE 6

Number of Gram blocks of type (j, k), $1 \leqslant j \leqslant 8$, $1 \leqslant k \leqslant j$,

in the interval $[g_{156{,}800{,}000}, g_{200{,}000{,}000})$

↓ j	k → 1	2	3	4	5	6	7	8	total
1	30,162,315								30,162,315
2	2,279,942 (50)	2,281,053 (50)	43 blocks with 0 0 zero-pattern 3 blocks with 2 2 zero-pattern						4,561,041
3	479,720 (47)	53,497 (5)	480,613 (47)						1,013,830
4	87,367 (46)	8,592 (4)	8,499 (4)	87,150 (45)					191,608
5	7,581 (38)	1,811 (9)	948 (5)	1,882 (9)	7,678 (39)				19,900
6	156 (12)	337 (27)	119 (10)	126 (10)	366 (29)	147 (12)			1,251
7	0	29	17	3	17	26	1		93
8	0	0	1*)	0	0	1*)	1*)	0	3

*)viz. B_n, for n = 175,330,804, 181,390,731 and 165,152,519.

In Table 6 we list the number of Gram blocks of type (j, k), $1 \leqslant j \leqslant 8$, $1 \leqslant k \leqslant j$, in the interval $[g_{156{,}800{,}000}, g_{200{,}000{,}000})$, as they were actually counted by the L R & W-program. On the line with $j = 2$ we also mention the numbers of Gram blocks of length 2 with zero-pattern "0 0" and those with pattern "2 2" which could, of course, neither be classified as type $(2, 1)$ nor as $(2, 2)$. The 43 blocks with "0 0"-pattern correspond to the exceptions to Rosser's rule in $[g_{156{,}800{,}000}, g_{200{,}000{,}000})$ and

the 3 blocks with "2 2"-pattern correspond to the exceptions of types 5 and 6 (cf. Table 2). The entries in parentheses give the approximate percentages with respect to the total number of blocks of length j, given in the final column.

Our main purpose in presenting this table is to render support to the L R & W-strategy of dealing with Gram blocks of length $j \geq 2$. The table shows that this strategy is successful for $2 \leq j \leq 5$. However, for $j \geq 6$ the missing two zeros show an increasing tendency to lie either in (g_{n+1}, g_{n+2}) or in (g_{n+j-2}, g_{n+j-1}). Only one of the 93 blocks of length $j = 7$ has its missing two zeros in one of the outer Gram intervals!

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