CMST (Early View) 1–13 (2022) DOI:10.12921/cmst.2022.0000014

The High Precision Numerical Calculation of Stieltjes Constants. Simple and Fast Algorithm

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Received: 6 June 2022; revised: 13 June 2022; accepted: 15 June 2022; published online: 25 June 2022

Abstract: We present a simple but efficient method of calculating Stieltjes constants at a very high level of precision, up to about 80 000 significant digits. This method is based on the hypergeometric-like expansion for the Riemann zeta function presented by one of the authors in 1997 [19]. The crucial ingredient in this method is a sequence of high-precision numerical values of the Riemann zeta function computed in equally spaced real arguments, i.e. $\zeta(1+\varepsilon), \zeta(1+2\varepsilon), \zeta(1+3\varepsilon), ...$ where ε is some real parameter. (Practical choice of ε is described in the main text.) Such values of zeta may be readily obtained using the PARI/GP program, which is especially suitable for this.

Key words: Riemann zeta function, Stieltjes constants, experimental mathematics, PARI/GP computer algebra system

I. Introduction: the Riemann ζ Function

Fundamental formulas in number theory are seldom numerically efficient. Although deep and absolutely precise, they may even hide the most important features of involved quantities. As a prominent example we consider the celebrated zeta function $\zeta(s)$ discovered by Euler in 1737 and published in 1744 [11] as a function of real variable and meticulously investigated by Riemann in the complex domain in his famous memoir submitted in 1859 to the Prussian Academy [21]:

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} , \qquad \mathrm{Re}(s) > 1. \tag{1}$$

This is a special case of a more general class of functions called Dirichlet series. It is divergent in the most interesting area of the complex plane, i.e., in the so called critical strip $0 \leq \mathrm{Re}(s) \leq 1$ where all complex zeros of zeta lie. However, as was shown by Riemann, the definition (1) does contain information about the zeta function on the entire complex plane but the process of analytic continuation must be used in order to reveal global behavior of this function. There is no universal procedure how to achieve this in practice and usually various ingenious tricks are required. For example, considering a simply alternating version of (1) leads to another Dirichlet series which is convergent for $\mathrm{Re}(s) > 0$ (except $s = 1$), i.e. also inside the critical strip:

$$\zeta(s) = \frac{1}{1-2^{1-s}} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^s} , \qquad \mathrm{Re}(s) > 0, \quad s \neq 1.$$

However, in order to obtain globally convergent representation for ζ one has to use more sophisticated techniques. We shall describe such an approach below.

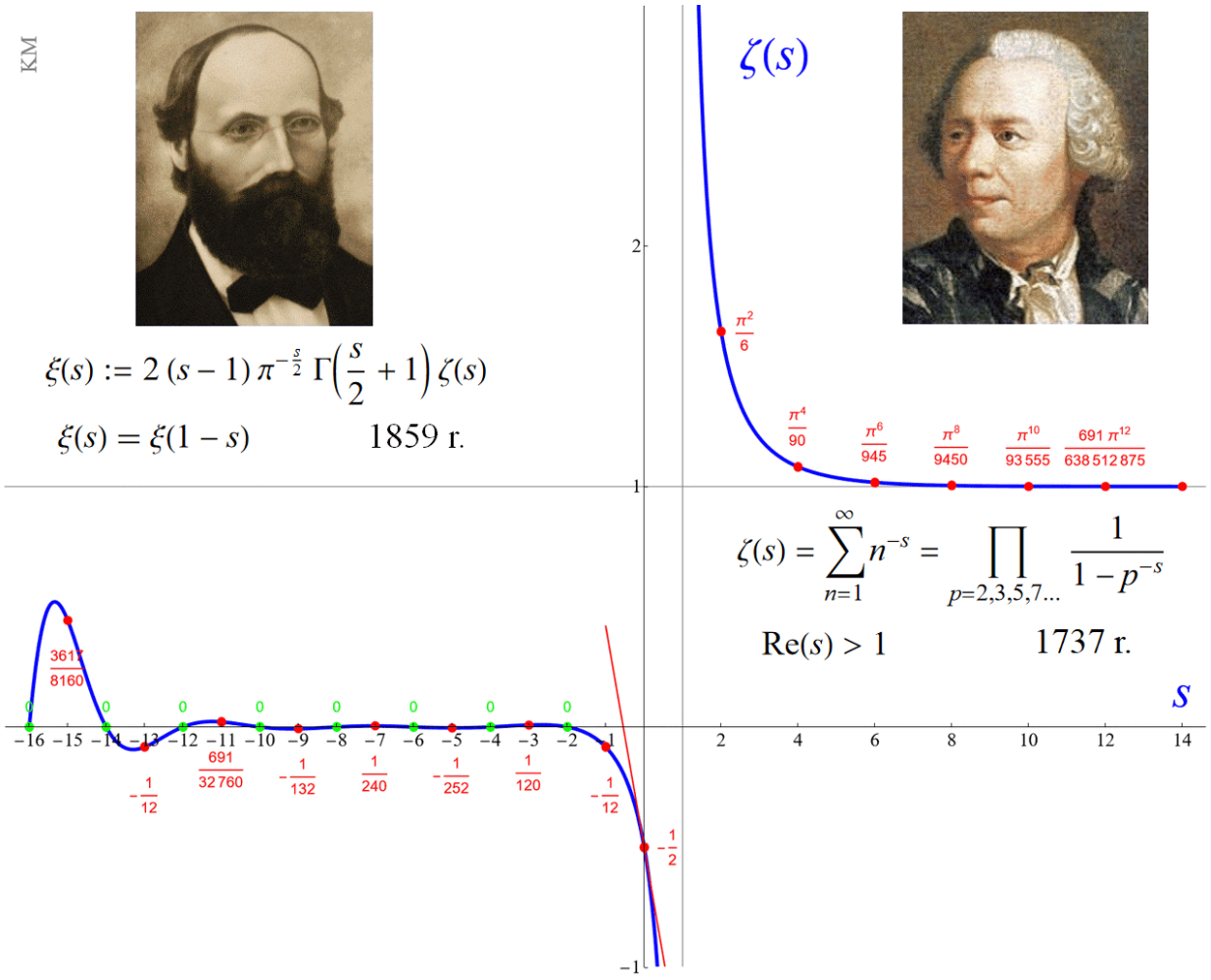

Fig. 1. Plot of the zeta function for real variable (blue curve). Euler discovered the zeta function in 1737 and found its deep connection with prime numbers [11] (see box on the right). But it was Riemann who in 1859 rigorously proved certain fundamental equation for it and made its analytical continuation to the entire complex plane, except for a single pole for $s = 1$ [21] (box on the left). Values of zeta for $s = 2n$, $n = 1, 2, \ldots$ were found by Euler in closed form (red dots). $\zeta(-2n) = 0$ are so called trivial zeros (green dots)

The Riemann zeta function contains the (heavily encoded) puzzle of the distribution of prime numbers. According to the famous saying by Paul Erdös (1913–1996), the solution to this puzzle may appear only "in millions of years, but even then it will not be complete, because in this case we are facing Infinity". We know, however, that this secret lies in the distribution of the zeros of the zeta function, i.e. the roots of the "simple" equation $\zeta(s) = 0$, on the complex plane. In 1859 Riemann hypothesized that *all* these roots (except for the so-called trivial ones) lie precisely on the line $\mathrm{Re}\, s = \frac{1}{2}$.

Despite the passage of more than 150 years and the persistent efforts of many top-class mathematical talents, the Riemann hypothesis remains unsettled. We simply do not know whether it is true or false. (Some think that it is undecidable.) Computer experiments based on billions of numerically calculated complex roots seem to confirm it. However, an exact proof still remains beyond the reach of mathematicians. It seems no one has even had a good idea of how to tackle this problem so far. Some have suggested that "new math" is needed, but this view is too vague to be of any practical help.

II. Stieltjes Constants

The Stieltjes constants are closely related to the Riemann zeta function, and since this function is extremely important in the analytical number theory, these constants are equally important.

Formulas for the Stieltjes constants may serve as another example of strict and deep but numerically inefficient formulas. These constants are essentially coefficients of the Laurent series expansion of the zeta function around its only simple pole at $s = 1$:

$$\zeta(s) = \frac{1}{s-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \gamma_n \,(s-1)^n \ . \qquad (2)$$

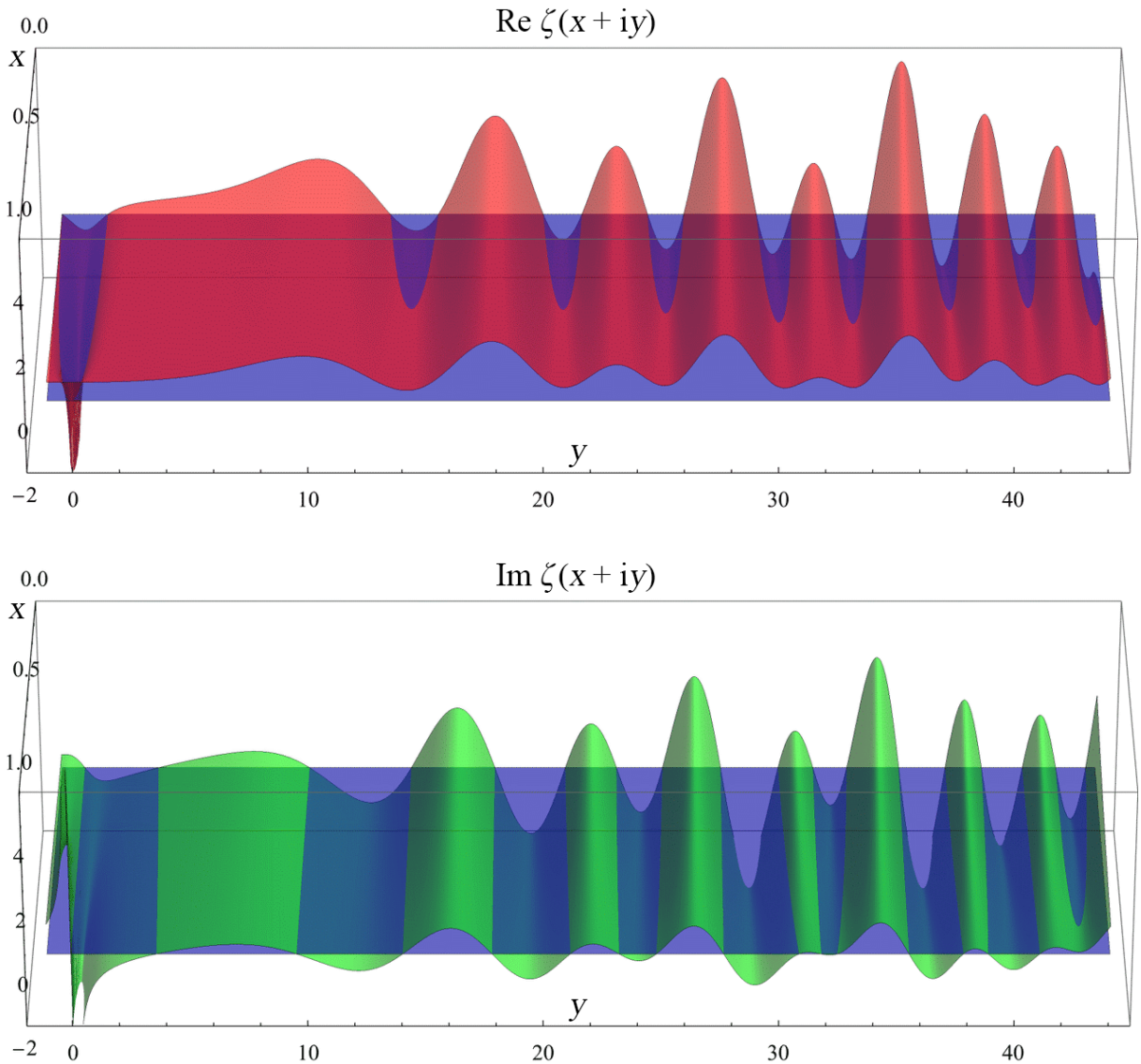

Fig. 2. The zeta function shows its essence and its true meaning only in the complex domain, and we owe knowledge about it to Riemann. The upper graph is the real part of the zeta function $\zeta(s)$, the lower graph is its imaginary part in the complex domain. The blue plane is the plane of the complex variable s

Primary definition of these fundamental constants was found by Thomas Jan Stieltjes and presented in a letter to his close friend and collaborator Charles Hermite dated June 23, 1885 [14]:

$$\gamma_n = \lim_{m\to\infty}\left(\sum_{k=1}^{m}\frac{(\ln k)^n}{k} - \frac{(\ln m)^{n+1}}{n+1}\right). \qquad (3)$$

When $n = 0$ the numerator in the first summand in (3) is formally 0^0 which is taken to be 1. In this case, (3) reduces simply to the well-known Euler-Mascheroni constant

$$\gamma_0 = \lim_{m\to\infty}\left(\sum_{k=1}^{m}\frac{1}{k} - \ln m\right),$$

which, roughly speaking, measures the rate of divergence of the harmonic series.

Effective numerical computing of the constants γ_n is quite a challenge because the formulas (3) are extremely slowly convergent. Even for $n = 0$, in order to obtain just 10 accurate digits one has to sum up exactly 12 366 terms whereas in order to obtain 10 000 digits (which is indeed required in some applications) one would have to sum up unrealistically large number of terms: nearly $5\cdot 10^{4342}$ which is of course far beyond the capabilities of the present day computers. For $n > 0$ the situation is still worse. Therefore we have to seek for other faster algorithms.

Due to the terribly slow convergence mentioned above, the progress in calculating the numerical values of Stielt-

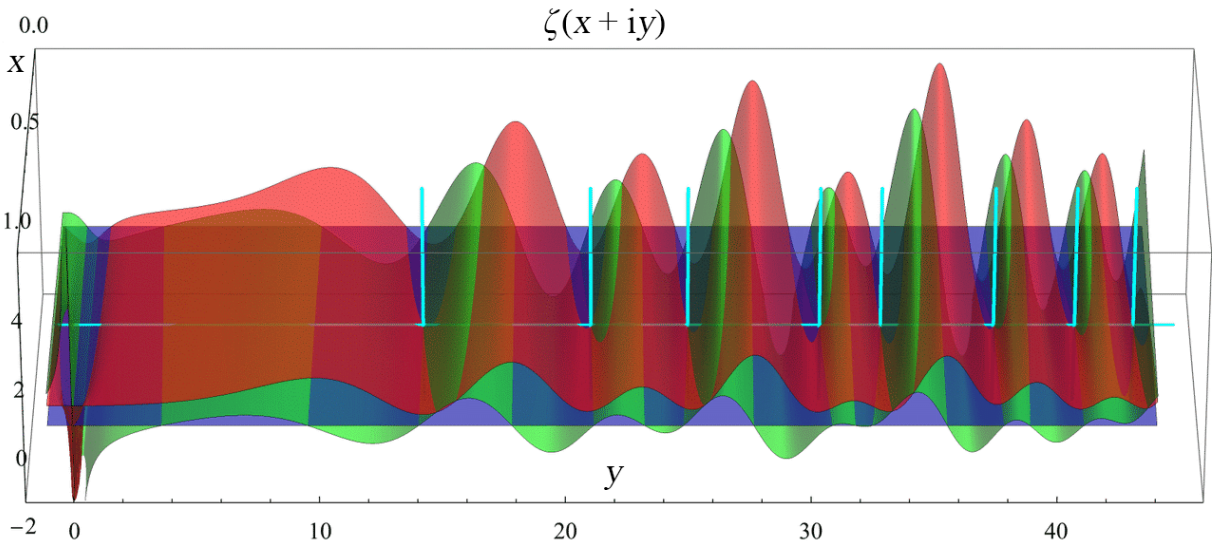

Fig. 3. Both surfaces shown in Fig. 2 intersect the plane of the complex variable s along certain irregular curves.After overlapping these surfaces, it turns out that these curves intersect themselves at certain points – these are the complex zeros of the zeta function (indicated by vertical blue lines). The Riemann hypothesis says that *all* these zeros are placed exactly on the line $\mathrm{Re}\, s = 1/2$

jes constants values was very slow. In his letter to Hermite, Stieltjes himself gave just two very inaccurate values for these constants γ_n (except for the then well-known Euler-Mascheroni constant γ_0):

$$\begin{aligned}\gamma_1 &= -0.072815(520)...\\ \gamma_2 &= -0.004(7)...\end{aligned}$$

(Here and below, digits in brackets are incorrect.) Two years later, in 1887, Jensen [15] gave eight values with nine significant digits:

$$\begin{aligned}\gamma_1 &= +0.072815845...\\ \gamma_2 &= -0.004845182...\\ \gamma_3 &= -0.000342306...\\ \gamma_4 &= +0.0000968(89)...\\ \gamma_5 &= -0.000006611...\\ \gamma_6 &= -0.000000332...\\ \gamma_7 &= +0.000000105...\\ \gamma_8 &= -0.000000009...\end{aligned}$$

Certain hope is in using integral representations of the Stieltjes constants. There are at least three such integrals:

- by directly applying Cauchy integral formula for derivatives to the Riemann zeta function we get:

$$\gamma_n = \frac{(-1)^n n!}{2\pi}\int_0^{2\pi} e^{-nit}\zeta\left(e^{it}+1\right)dt, \qquad (4)$$

- by Franel, 1895 [13]

$$\gamma_n = \frac{1}{2}\delta_{n,0} + \\ +\frac{1}{i}\int_0^\infty \frac{dt}{e^{2\pi t}-1}\left[\frac{(\ln(1-it))^n}{1-it} - \frac{(\ln(1+it))^n}{1+it}\right], \qquad (5)$$

- by Blagouchine [7, 8]

$$\gamma_n = \frac{\pi}{2(n+1)}\int_{-\infty}^{\infty}\frac{\left(\ln\left(\frac{1}{2}\pm it\right)\right)^{n+1}}{(\cosh \pi t)^2}dt. \qquad (6)$$

Using these integral representations one can, for example with the help of the procedure **NIntegrate** which is built in

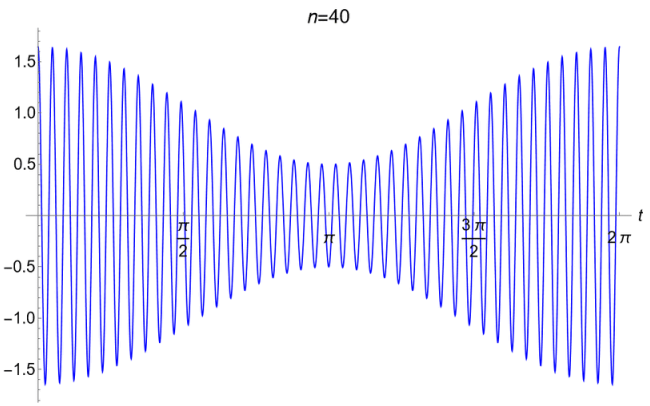

Fig. 4. Real part of the integrand (4) which contributes to the value of γ_{40} (integrating the imaginary part which is antisymmetric with respect to $t = \pi$ gives zero). The number of oscillations grows as n. Therefore, for large n the numerical integration procedure cannot properly estimate this integral

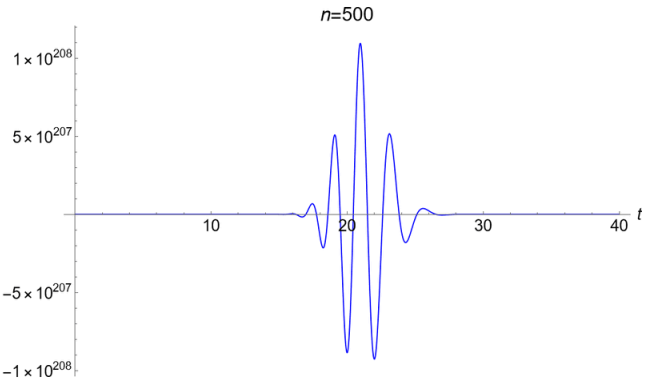

Fig. 5. Real part of the integrand in (6). The number of oscillations grows with n but, contrary to the case (5), their amplitude also increases very quickly with n

Wolfram *Mathematica*, calculate γ_n up to $n = 1000$ with precision of several hundred significant digits in a reasonable computer time. However, increasing n and/or the working precision parameter in **NIntegrate** produces an error message in the *Mathematica* output. This can be easily understood when looking at the behavior of the integrand of (4) which for growing n contains more large oscillations.

There are also several series representations of Stieltjes constants, e.g. such as this given by I. Blagouchine [7, 8]

$$\gamma_n = -\frac{1}{n+1}\sum_{k=0}^{\infty}\frac{1}{k+1}\sum_{j=0}^{\infty}(-1)^j\binom{k}{j}\log^{n+1}(j+1)\,, \tag{7}$$

and another one found by M. Coffey [10] (Corollary 13, with misprint)

$$\gamma_n = -\frac{2}{3}n!\sum_{i=1}^{n}\frac{B_{n-i+1}c^{n-i}}{i!(n-i+1)!}h_i - \frac{2}{3c(n+1)}h_{n+1} - \frac{B_{n+1}}{n+1}c^{n+1}, \tag{8}$$

where

$$\begin{aligned} c &\equiv \ln 2, \\ h_i &\equiv \sum_{k=1}^{\infty}3^{-k}\sum_{j=1}^{k}\frac{(-1)^j 2^j}{j+1}\binom{k}{j}\ln^i(j+1). \end{aligned}$$

Unfortunately, both (7) and (8) are also very slowly convergent and rather useless in numerical investigations – contrary to what Coffey claims: "The expression may be attractive for some computational applications because it exhibits even faster convergence" (see [10], p. 23).

Significant progress took place in 1984-1985 with the work of Ainsworth and Howell [3, 4] who received a grant from NASA and probably used a computer. (It could be an analog machine, but they did not disclose the technical details of their calculations.) They used another integral representation of the Stieltjes constants and with the help of the Gauss numerical integration formula tabulated 200 initial γ_n with just 10 significant digits each. They also calculated a few selected values of γ_n for larger $n = 500, 1000, 1500, 2000$. In the latter cases, some of their digits are incorrect.

In 1992, Keiper[1] published an effective algorithm for calculating Stieltjes constants. Keiper's algorithm was later implemented in *Mathematica* [17]. (However, no technical details about this algorithm can be found in *Mathematica* documentation except for a concise statement that it "uses Keiper's algorithm based on numerical quadrature of an integral representation of the zeta function and alternating series summation using Bernoulli numbers".)

An efficient but rather complicated method based on Newton-Cotes quadrature has been proposed by Kreminski in 2003 [18]. This was a real achievement since Kreminski computed γ_n up to $n = 3000$ with several thousand digits and was able to observe certain interesting structures in the distribution of γ_n.

Quite recently (2013) Johansson presented a particularly efficient method [16]. He calculated a new, impressive, record-breaking value of γ_n for $n = 100\,000$. Later (2018), in collaboration with Blagouchine, Johansson reached the next record values: $n = 10^{10}, 10^{15}$ and 10^{100}.

In the present paper yet another method of computing Stieltjes constants will be described which, we believe, is perhaps not as efficient as Johansson's approach, yet it is much simpler and it may be easily and quickly used in practical calculations for obtaining γ_n up to $n \sim 30\,000$ with precision $\sim 80\,000$ significant digits.

III. Riemann Zeta Representation

In 1997, it was shown by one of the present authors [19, 20] that the Riemann zeta function may be expressed as

$$\zeta(s) = \frac{1}{s-1}\left[A_0 + \left(1-\frac{s}{2}\right)A_1 + \left(1-\frac{s}{2}\right)\left(2-\frac{s}{2}\right)\frac{A_2}{2!} + \ldots\right] = \tag{9}$$

$$= \frac{1}{s-1}\sum_{k=0}^{\infty}\frac{A_k}{k!}\prod_{i=1}^{k}\left(i-\frac{s}{2}\right) = \tag{10}$$

$$= \frac{1}{s-1}\sum_{k=0}^{\infty}\frac{\Gamma\left(k+1-\frac{s}{2}\right)}{\Gamma\left(1-\frac{s}{2}\right)}\frac{A_k}{k!} = \tag{11}$$

$$= \frac{1}{s-1}\sum_{k=0}^{\infty}\left(1-\frac{s}{2}\right)_k\frac{A_k}{k!}\,, \qquad s\in\mathbb{C}\backslash\{1\}, \tag{12}$$

[1] Jerry B. Keiper (1953–1995) worked for Wolfram Research and was an active contributor to *Mathematica*. He developed, among others, many effective algorithms for numerical computation of special functions. He died tragically returning from work on his bike, hit by a car.

where

$$A_k = \sum_{j=0}^{k} (-1)^j \binom{k}{j} (2j+1)\zeta(2j+2) = \quad (13)$$

$$= \frac{1}{2}\sum_{j=0}^{k} \binom{k}{j} (2j+1)\frac{(2\pi)^{2j+2} B_{2j+2}}{(2j+2)!}\,, \quad (14)$$

$(x)_k$ is the Pochhammer symbol and B_n is the n^{th} Bernoulli number [2].

The main idea behind this approach is to remove the single pole of the zeta function multiplying it by $s-1$ and then to fix values of this entire function in an infinite number of *equally spaced* real points, which corresponds simply to interpolation with nodes. Note that in (9)–(12) these points are precisely the points in which, as shown by Euler, zeta values are known exactly, i.e. $s = 2, 4, 6, ...$ Indeed, series (9) truncates in these points and gives appropriate exact values.

It may be shown that this representation is globally convergent. Real coefficients A_k expressed as an alternating binomial sum are in fact combinations of Bernoulli numbers and even powers of π. On the other hand, $(-1)^k A_k$ are simply consecutive finite step derivatives of some entire function, namely $(2s+1)\zeta(2s+2)$ that involves these points in which, as Euler had shown, zeta is explicitly known.

Considered as a sort of polynomial interpolation with fixed nodes the expansion (9) might appear trivial. However, this is not the case since many "simple" functions, e.g. Lorentz function $1/(1+x^2)$, exhibit nasty phenomenon known as the Runge effect: oscillations between fixed nodes growing when the number of terms in the series increases. This behavior may be cured using *unequally* spaced nodes, so called Chebyshev nodes, but this in turn spoils the very idea of (9), which naturally leads to Pochhammer symbols. From this point of view the global validity of (9) is equivalent to the following simple statement: the regularized Riemann zeta function $(s-1)\zeta(s)$ does not exhibit Runge phenomenon.

The original proof of (9) contained a gap [19]. Rigorous proof was given in 2003 by Báez-Duarte[2] [5] who also presented certain simple and esthetic criterion for the Riemann Hypothesis based on expansion (9) [6]. Another very short and particularly elegant proof of (9) using Carlson theorem was given by Flajolet and Vepstas in 2007 [12]. Later a whole class of similar zeta representations was published [20].

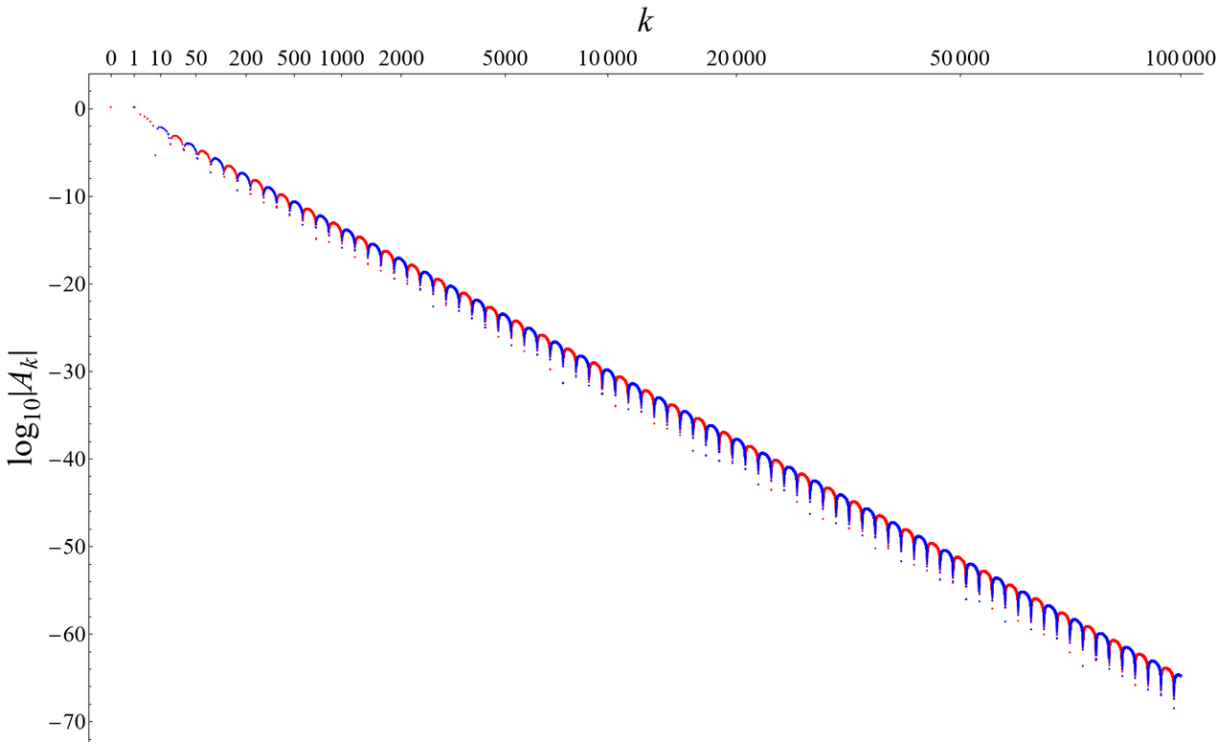

Fig. 6. Curious behavior of the coefficients A_k. given by (13). There are unexpected oscillations with slowly diminishing frequency (roughly as $k^{-2/3}$) and nearly exponentially diminishing amplitude. Note that the k-axis is scaled as $\sqrt[3]{k}$. Red points correspond to positive values of A_k and blue to negative ones

[2] The prominent Venezuelan mathematician Luis Báez-Duarte (1938–2018), educated in the USA, Massachusetts Institute of Technology, and working at the Instituto Venezolano de Investigaciones Científicas (IVIC) in Caracas, was a close friend and collaborator of one of the authors (K.M.). Although they had never met in person, from 2003 until Luis' death, they corresponded regularly, mainly on mathematical topics, but also on general topics related to literature, history, politics, etc.

Coefficients A_k tend to zero sufficiently fast, which is crucial to assure the global convergence of the series (9). However, their detailed behavior with growing k is quite striking as can be seen on a logarithmic plot with the k-axis rescaled as $\sqrt[3]{k}$. More precisely: they exhibit curious and unexpected oscillatory behavior with both amplitude and frequency decreasing when k tends to infinity (see Fig. 6).

This peculiar behavior "cries for explanation" as stated in [12] (p. 2). Using the saddle point method one can show that for k tending to infinity the following asymptotics holds (K. Maślanka, *An Asymptotic Expansion for the Stieltjes Constants*, in preparation):

$$A_k \sim \frac{4\pi^{3/2}}{\sqrt{3\kappa}} \exp\left(-\frac{3}{2}\kappa+\frac{\pi^2}{4\kappa}\right)\cos\left(\frac{4\pi}{3}-\frac{3\sqrt{3}}{2}\kappa-\frac{\sqrt{3}\pi^2}{4\kappa}\right), \tag{15}$$

where

$$\kappa \equiv \pi^{3/2}\sqrt[3]{k}\,,$$

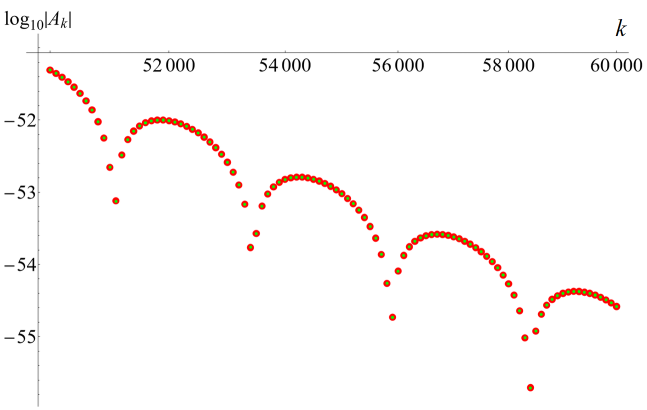

Fig. 7. Asymptotic formula (15) works quite well: red dots represent exact values of A_k as given by (13) whereas smaller green dots are calculated from (15)

Coefficients A_k also obey certain simple algebraic identities which stem directly from trivial zeros of zeta and from the fact that $\zeta(0) = -\frac{1}{2}$. Indeed, substituting in (9) $s = 0, -2, -4, -6, \ldots$ and making use of elementary properties of the Euler gamma function we successively get:

$$\begin{aligned}
\sum_{k=0}^{\infty} A_k &= \frac{1}{2}\,, \qquad (16)\\
\sum_{k=0}^{\infty}(k+1)A_k &= 0\,,\\
\sum_{k=0}^{\infty}(k+1)(k+2)A_k &= 0\,,\\
\sum_{k=0}^{\infty}(k+1)(k+2)(k+3)A_k &= 0\,,\\
&\ldots
\end{aligned}$$

After some simple manipulations we finally get:

$$\sum_{k=0}^{\infty} k^n A_k = \frac{(-1)^n}{2}\,, \qquad n = 0, 1, 2, \ldots \tag{17}$$

with the convention $k^n = 1$ when $k = n = 0$. Unfortunately, due to slow convergence of (17) when n is large, these identities cannot be effectively used to calculate A_k. Another interesting identity follows from $\zeta'(0) = -\frac{1}{2}\log(2\pi)$:

$$\sum_{k=0}^{\infty} A_k H_k = 1 - \log(2\pi), \tag{18}$$

where $H_k \equiv \sum_{i=1}^{k} \frac{1}{i}$ is the k^{th} harmonic number.

IV. Algorithm for Calculating Stieltjes Constants

The particular choice of nodes in $s = 2, 4, 6, \ldots$ in the expansion (9), albeit the most natural, is by no means the only one. One only requires that the prescribed points be strictly equally spaced. For the purpose of present calculations we choose the following sequence of points:

$$1, 1+\varepsilon, 1+2\varepsilon, 1+3\varepsilon, \ldots$$

where ε is a certain real, not necessarily small number.

More precisely, define certain entire function f as:

$$f(s) := \begin{cases} \zeta(s) - \frac{1}{s-1}\,, & s \neq 1,\\ \gamma\,, & s = 1, \end{cases} \tag{19}$$

where γ is the Euler constants which stems from the appropriate limit. Then, instead of (11), we have

$$f(s) = \sum_{k=0}^{\infty} \frac{\Gamma\left(k - \frac{s-1}{\varepsilon}\right)}{\Gamma\left(-\frac{s-1}{\varepsilon}\right)} \frac{\alpha_k}{k!}\,,$$

with

$$\alpha_k = \sum_{j=0}^{k} (-1)^j \binom{k}{j} f(1+j\varepsilon). \tag{20}$$

Note that coefficients α_k depend on ε but for simplicity we shall temporarily drop this dependence in the notation. Now directly from (2) we have:

$$\gamma_n = (-1)^n \frac{d^n}{ds^n} f(s)\bigg|_{s-1}\,.$$

Then, after some elementary calculations we get the main result of the present paper:

$$\boxed{\gamma_n = \frac{n!}{\varepsilon^n} \sum_{k=n}^{\infty} \frac{(-1)^k}{k!} \alpha_k S_k^{(n)}}\,, \tag{21}$$

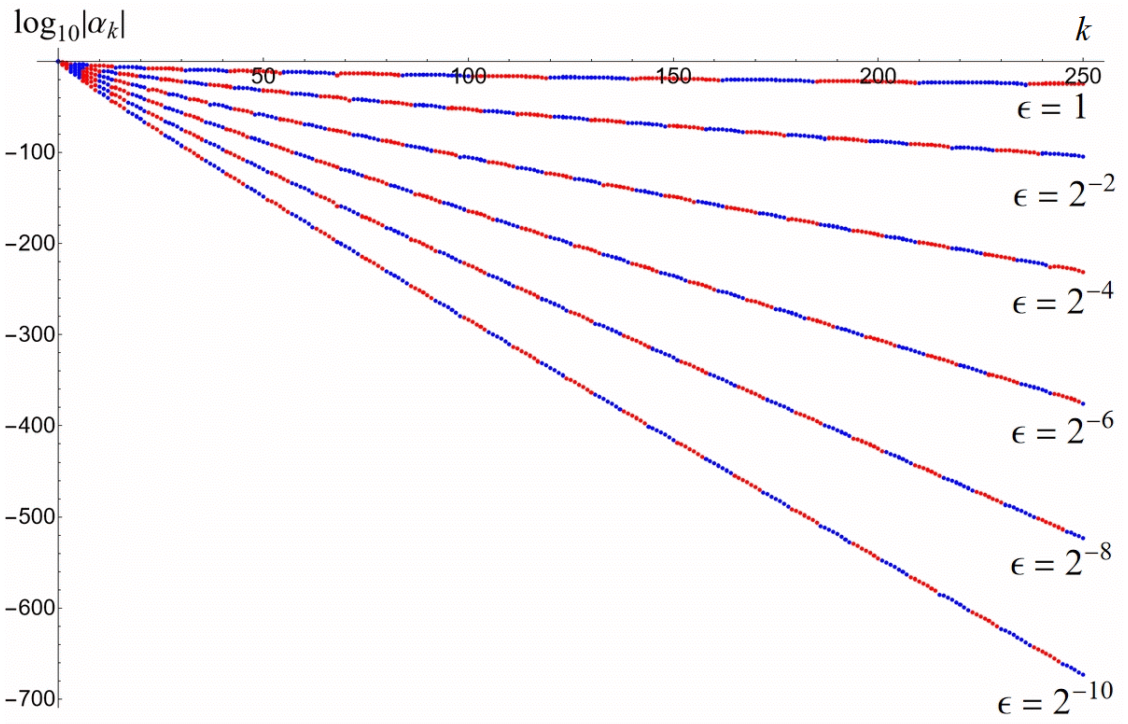

Fig. 8. Behavior of coefficients α_k given by (20) for different choices of the parameter ε

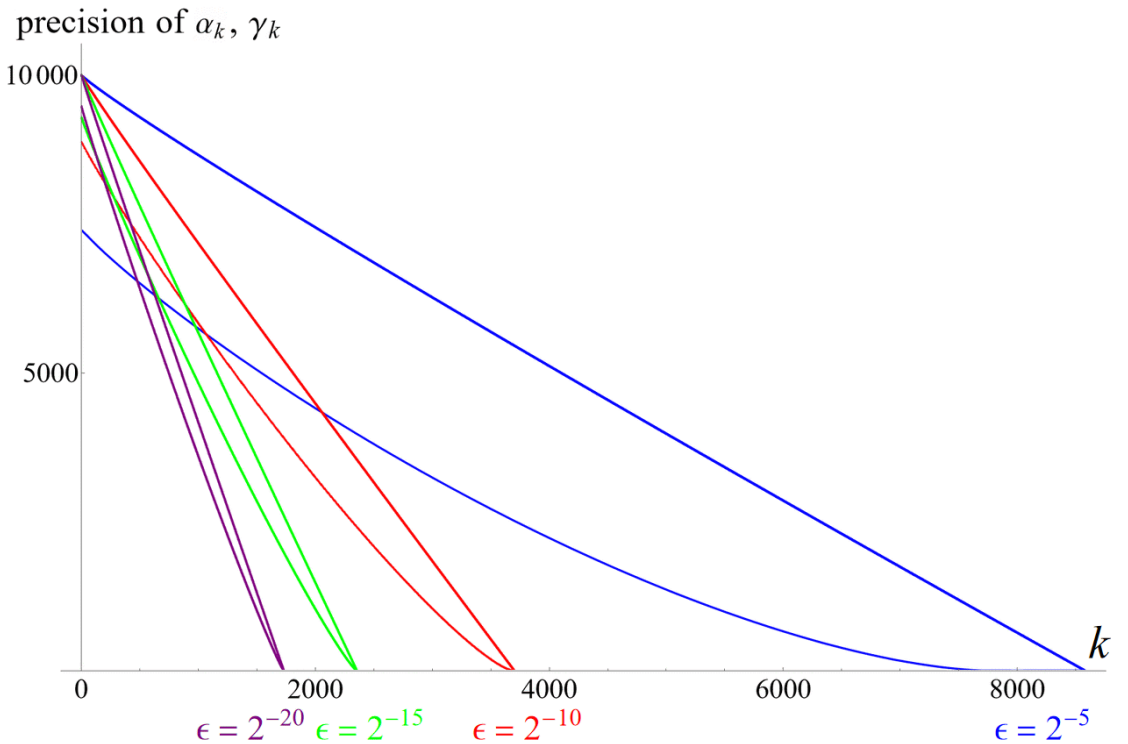

Fig. 9. Plots of precision of a_k and γ_k versus k for precision of the precomputed equidistant zeta values equal to 10 000 significant digits and for four values of the auxiliary parameter ε: blue – ε^{-5}, red – ε^{-10}, green – ε^{-15}, purple – ε^{-20}. For each color the upper, nearly straight line segment corresponds to precision of α_k, and the piece of a curved line of the same color corresponds to the precision of γ_k. Since precision of α_k diminishes with growing k, for any given value of ε there always exists a specific, unambiguous value of index k_0 such that for all $k > k_0$ precisions of all α_k are numerically zero. Hence in the formula (23) it is enough to sum only up to this value

where $S_k^{(n)}$ are signed Stirling numbers of the first kind. Note that in the literature there are different conventions concerning denotation and indices of Stirling numbers which may be confusing. Here, following [2], we shall adopt the following convention involving the Stirling numbers and the Pochhammer symbol:

$$(x)_k \equiv \frac{\Gamma(k+x)}{\Gamma(x)} = \prod_{i=0}^{k-1}(x+i) =$$
$$= (-1)^k \sum_{i=0}^{k}(-1)^i S_k^{(i)} x^i = \sum_{i=0}^{k}\left|S_k^{(i)}\right| x^i \ .$$

Denoting

$$\beta_{nk} \equiv \frac{n!}{k!}\frac{S_k^{(n)}}{\varepsilon^n} \ ,$$

we can rewrite (21) as formally an infinite matrix product

$$\gamma_n = \sum_{k=n}^{\infty} \beta_{nk}\, \alpha_k \ . \tag{22}$$

The summation over k starts from n since $\beta_{nk} \equiv 0$ for $k < n$. Precision of α_1 is equal to precision of precomputed values of $f(s)$ given by (19) in equidistant nodes. When k grows the precision of consecutive α_k almost linearly tends to zero. Thus there always exists a certain cut-off value of $k = k_0$. Therefore, the summation in (22) should be performed to this value:

$$\gamma_n = \sum_{k=n}^{k_0} \beta_{nk}\, \alpha_k \ . \tag{23}$$

(Adding more terms is inessential. In other words, one cannot compute γ_n for $n > k_0$. In order to perform this, one should increase precision of the precomputed values of $f(s)$ which would in turn proportionally increase k_0, see Fig. 9 for detailed description.)

As pointed earlier ε need not to be small; however, choosing smaller ε greatly accelerates convergence of the series. Yet, it turns out that smaller ε implies smaller k_0. What is really important is that all significant digits of γ_n obtained from the finite sum (23) are correct.

Of course, γ_n eventually does not depend on a particular choice of ε, as expected, although α_k as well as the rate of convergence of (21)–(23) does. In fact series (21) converges for any value of $\varepsilon > 0$ but the rate of convergence becomes extremely small for $\varepsilon \sim 1$. On the other hand, the smaller ε, the faster the rate of convergence. However, since α_k also depends on ε, choosing a smaller value for ε requires higher precision of precalculated values of $f(s)$ which in turn may be very time consuming. Hence, an appropriate compromise in choosing ε is needed.

Formula (23) is particularly well-suited for numerical calculations. Typically the algorithm has three simple steps:

1. Tabulating function (19) for equidistant arguments $1 + j\varepsilon$, i.e. $f(1 + j\varepsilon), j = 0, 1, 2, ...$ This is most time-consuming and requires appropriate choice of parameter ε. (In our case, we have chosen the value $\varepsilon = 2^{-10}$.) What seems most convenient for these calculations is a small but extremely efficient program PARI/GP which has implemented particularly optimal zeta procedure. We used the Cyfronet Prometheus computer where calculating single value of $f(s)$ with 80 000 significant digits requires about 10–15 minutes each. Since this procedure may be easily parallelized, in order to compute more than 30 000 values of f we started several dozen independent routines (each calculating a few thousands values of f).
2. Calculating α_k using (20) and the precomputed values of f.
3. Calculating Stieltjes constants using (21).

(Contrary to the above steps 2. and 3., step 1 requires a powerful computer, whereas steps 2 and 3 can be quickly performed on a typical PC.) It should be emphasized that with the α_k coefficients properly calculated, obtaining γ_n requires only a dozen or so minutes on a very modest PC machine. One property of the result (21) should again be stressed out: all digits of γ_n obtained from (23) are significant and reliable.

Step 1 was achieved using the following PARI code:

```
\g4
\p 80000;
default(parisizemax,1000000000);
allocatemem(1000000000);
eps=2^-10;
f(s)=if(s-1,zeta(s)-1/(s-1),Euler);
for(j=0,32000,write("zeta.dat","{",
    1+j*eps,",",f(1+j*eps),"},"));
```

Acknowledgment

This research was partly supported by PL-Grid Infrastructure and performed on the Prometheus multicore supercomputer, Cyfronet, Kraków. The kind and patient willingness to help and professional technical advice from the members of the Cyfronet team (Maciej Czuchry and Andrzej Dorobisz from High Performance Computing Software Department) when starting the project were very helpful. The authors of the Pari/GP computer algebra system (Bill Allombert and Karim Belabas) put a lot of effort into correcting the persistent error in the calculation of the Riemann zeta function for the great accuracies that were crucial to the presented algorithm. Finally, K.M. is grateful to Artur Jasiński for paying attention to formulas (5) and (6) as well as works [13] and [15].

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Appendix: Struggling with Certain PARI Bug

Common experience shows that there are no computer programs, especially larger ones, which – in certain specific and usually unpredictable situations – would not exhibit misbehavior. Computer program errors, according to the old tradition called "bugs", are usually an integral part of each program. Of course, program developers, or rather the large development teams that create them, spare no effort to ensure that their products are error-free. However, it is virtually impossible to remove them completely. In addition, professional computer programs are constantly developed and expanded, sometimes over many years, and new functions are added in subsequent versions, often at the explicit request of users. In this way, while previous bugs are removed, new bugs are inevitably added, although, of course, this happens unknowingly. The key role here is played by the fruitful cooperation of program users with their developers: numerous users scattered all over the world, solving their own specific problems, at the same time intensively test programs and provide their developers with relevant information about undesirable behavior of their products.

A sentence from a letter written by a PARI/GP user is particularly significant: "I hope you and your collaborators will be able to eliminate the bugs [...] in the forthcoming (final?) release of PARI" (April 1997). More than a quarter of a century has passed since then. PARI is growing, has a faithful group of users (mainly mathematicians dealing with the number theory), new functions and procedures are added, but the list of "bugs" does not decrease at all. It is instructive to look at the page: link[3], illustrating the intense and fruitful interaction of PARI users with its creators. For someone unfamiliar with the essence of computer programs, the sentence from the above-quoted letter sounds like the proverbial "wishful thinking". It is naive and unrealistic, although it was sent in good faith. The aforementioned "final version" of the program is an unattainable goal to which one can, at best, "approach asymptotically". It is also worth adding that this sentence was rightly placed on the PARI website with a meaningful title: "Fun!".

When testing the algorithm described in this article, we came across a surprising error in the numerical computation of the fundamental Riemann zeta function, which is built into PARI. As mentioned earlier, the presented algorithm requires "input" zeta values of great precision; in our case, we chose 80 000 significant digits. It was a kind of compromise between relatively high precision and reasonable computation time (several weeks on many cores of the Prometheus supercomputer

[3] https://pari.math.u-bordeaux.fr/cgi-bin/pkgreport.cgi?pkg=pari

in Cyfronet in Cracow. Probably no one has methodically tested PARI for calculations of the Riemann zeta with such great precision before.

The choice of PARI – a small (in the command-line version only about 12 MB) dedicated to calculations in the number theory as a tool to obtain the value of the zeta function – resulted from the high speed of calculations: several times greater than, for example, *Mathematica* (size of installation files over 4 GB). Unexpectedly tt turned out that the result file of the necessary numerical values in the form of the array $\{1 + j\varepsilon, f(1 + j\varepsilon)\}$ contained incorrect digits in the range of index j from 11 201 to 12 401.

Of course, finding those digits that were wrong among more than 2.5 billion digits was quite a challenge. It was a very tedious and frustrating job, like looking for the proverbial needle in a haystack. But it was even more challenging to figure out the very cause of this error. In the first case, some properties of the α_k coefficients proved to be helpful. In the second case, professional help of the PARI program developers turned out to be indispensable.

The first sign of the presence of these erroneous digits was that the coefficients α_k calculated from these values, instead of rapidly (exponentially) decrease to zero with the increase of the index k, drastically changed its behavior, see Fig. A1.

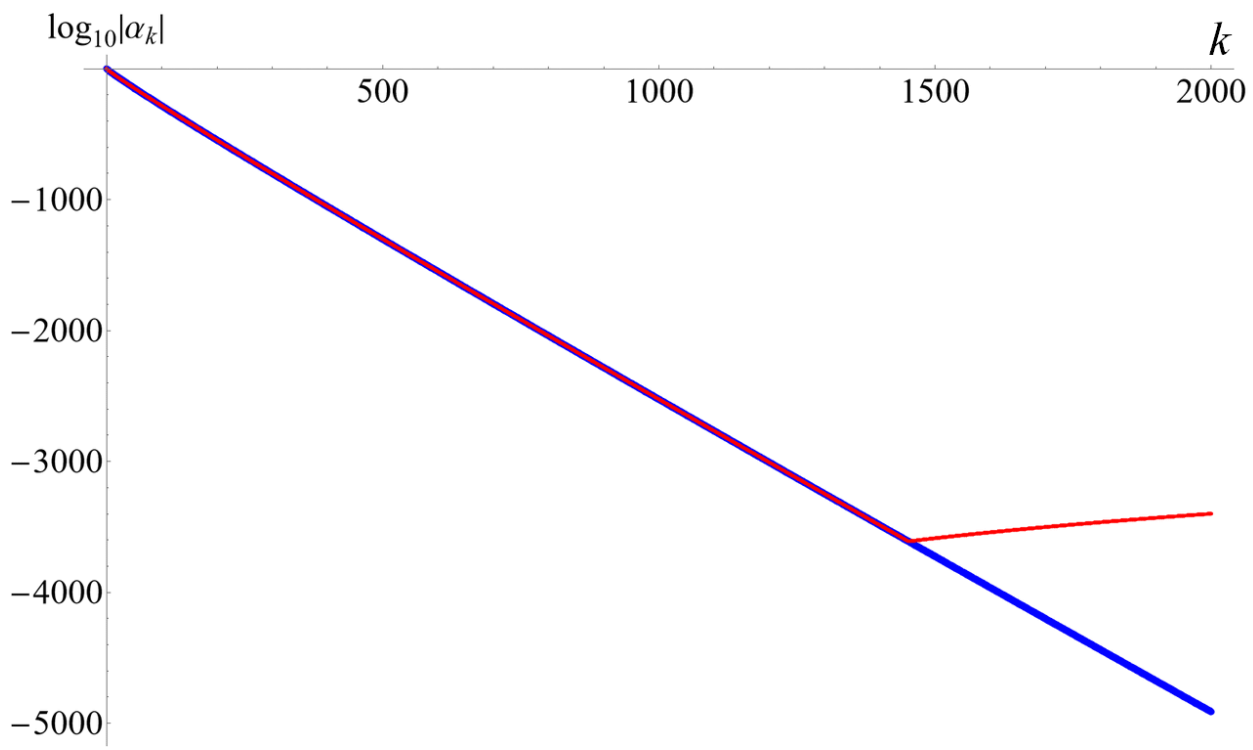

Fig. A1. Coefficients α_k given by (20) are extremely sensitive to even one wrong digit in the calculated value of the zeta function, even at a very distant place of its decimal expansion. The figure illustrates a sudden change in the behavior of the α_k coefficients (red line) when in the correct value of the regularized zeta function $f(1 + \varepsilon j)$ for $j = 1000$ only single digit is replaced with another one that differs from the correct one just by 1. The replaced digit might be in a very remote significant place (in this case it was on position 4000 after the decimal point), and yet α_k would "feel" and reveal that change anyway

Since the (regularized) zeta function, however complicated and mysterious, is a regular function, the successive finite differences of equidistant values of this function from the above-mentioned table $f(1 + j\varepsilon)$ should lie on a smooth curve. The tests performed with the use of the Mathematica procedure **Differences** that calculates successive finite differences revealed that for the above-mentioned values of index j and with the order of these differences about 400, disturbing oscillations appeared instead of a sequence of points lying along a smooth curve, see Fig. A2.

Intensive and very tedious tests, requiring great patience, time and computer resources, lasted for several weeks and were carried out with professional and very kind cooperation of employees of the Cyfronet Computer Center in Kraków (administrators of the Prometheus supercomputer). In order to eliminate the potential causes of generating wrong digits, we tested newer and newer development versions of PARI released daily. We used two different compilers (Intel icc 19.1.1.217 and GNU gcc version 4.8.5 20150623). We have compiled PARI in serial and parallel version (threading engine: pthread, mpi, single). Additionally, for the parallel version, we also ran single-core jobs to rule out the PARI "parfor" command as

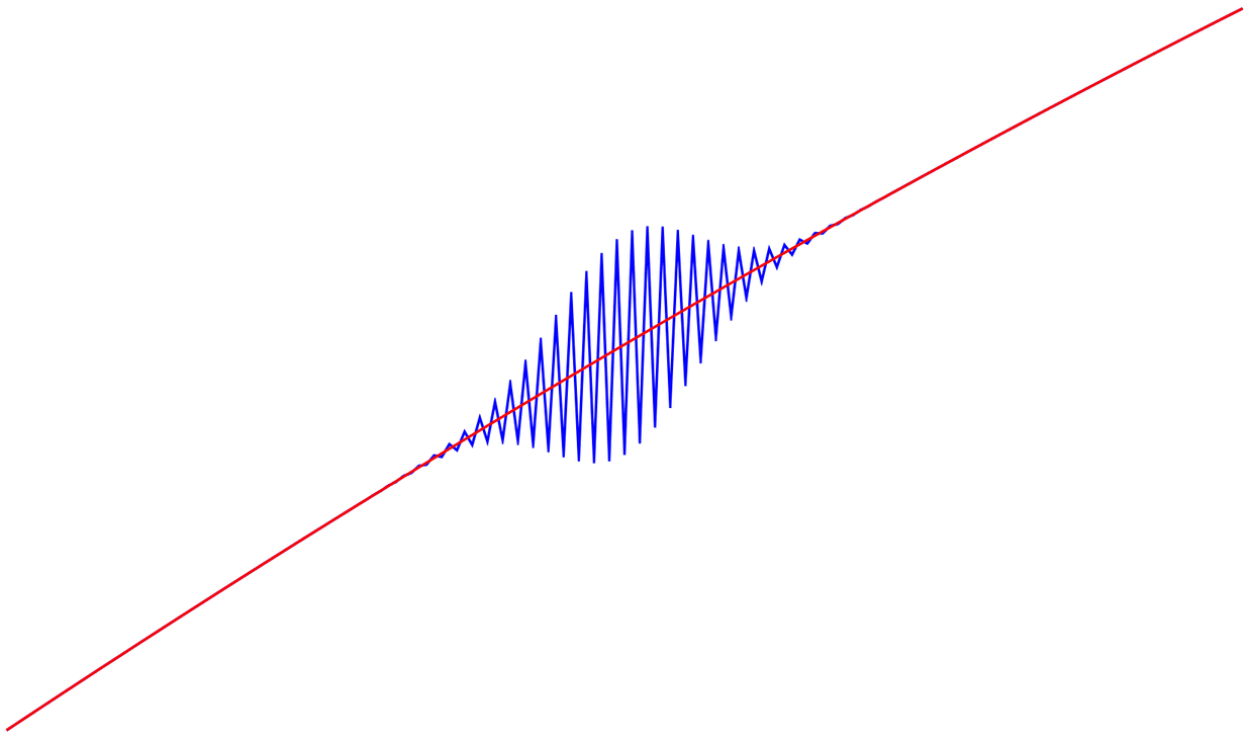

Fig. A2. Wolfram Mathematica procedure **Differences[*list*,*n*],** which gives the n^{th} differences of a given list, when applied to the list of "contaminated" data of the function $f(1+j\varepsilon)$ reveals that some digits are wrong. When the integer parameter n is sufficiently large then even a single wrong digit differing from the proper one by unity produces oscillations instead of a smooth distribution of points. In this case one had to use $n = 400$ to reveal the error. (In the above graph, both axes have been removed as they are irrelevant to demonstrate the effect described)

a possible source of the problem. We used different operating systems (Linux and Windows 10), different versions of Linux cores (x86-64, x86-64 / GMP-6.2.1, x86-64 / GMP-6.0.0) and different types of processors (Intel and AMD). We compared the obtained numbers with the results obtained with Wolfram Mathematica on PCs with AMD and Intel processors (these calculations took several times longer than with PARI). We additionally performed a series of calculations for precision from 30 000 to 90 000 in 10 000 steps and from 71 000 to 89 000 in 1000 steps. It turned out that the wrong numbers appeared at 174 decimal places only for the precision of 74 000 and 80 000.

The results of these tests were successively (from August 2021 to December 2021) delivered to the authors of the PARI program, who made appropriate corrections in the program code. (Incidentally, the first such correction did not remove the error; it appeared again but in a different range of index j, and even worse, i.e. for more significant digits of the Riemann zeta function...)

In the end, it turned out that the cause of this error was simply in the PARI-implemented procedure for computing the value of the zeta function which uses the classical Euler-Maclaurin algorithm. Specifically, the values of the Bernoulli numbers required to compute the zeta function were rounded unnecessarily. It was due to double roundings occurring when caching Bernoulli numbers, because of too frequent precision reductions. This bug did not affect the low precision computations, but was particularly bothersome with the algorithm described here. More details can be found here: link[4].

It should be emphasized that when computing the zeta function, PARI first computes and tabulates the appropriate Bernoulli numbers, according to the Euler-Maclaurin formula. During this stage of the calculations, which – depending on the precision set at the beginning – sometimes takes several hours, the results do not start to appear, and the program pretends that it has "hung".

The revised version of the program finally appeared at the end of December 2021. From that moment, having the necessary and reliable numerical data, i.e. the high precision (regularized) zeta values, we were able to return to purely mathematical problems and continue the main project of calculating the Stieltjes constants.

Finally, it should be emphasized once again that the main advantage of the algorithm for calculating important Stieltjes constants presented herein is its mathematical simplicity and numerical efficiency. Moreover, it can be a convenient starting

[4] https://pari.math.u-bordeaux.fr/cgi-bin/bugreport.cgi?bug=2311

point for deriving certain new asymptotic expansion for these constants, both more accurate and simpler than several expansions known in the literature. This will be the topic of another publication (K. Maślanka, *An Asymptotic Expansion for the Stieltjes Constants*, in preparation).

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 DOI:10.12921/cmst.2022.0000014