Convergence Acceleration Techniques

U. D. Jentschura[‡]*, S. V. Aksenov**, P. J. Mohr***, M. A. Savageau**, and G. Soff*

* Institute of Theoretical Physics, Dresden University of Technology, 01062 Dresden, Germany, jentschura@physik.tu-dresden.de
** Department of Microbiology and Immunology, The University of Michigan, Ann Arbor, MI 48109, USA, aksenov@umich.edu
*** National Institute of Standards and Technology, Mail Stop 8401, Gaithersburg, MD 20899, USA, mohr@nist.gov

ABSTRACT

This work describes numerical methods that are useful in many areas: examples include statistical modelling (bioinformatics, computational biology), theoretical physics, and even pure mathematics. The methods are primarily useful for the acceleration of slowly convergent and the summation of divergent series that are ubiquitous in relevant applications. The computing time is reduced in many cases by orders of magnitude.

Keywords: Computational techniques, numerical approximation and analysis.

1 CONVERGENCE ACCELERATION (A BRIEF OVERVIEW)

What does it mean to "accelerate convergence"? The answer is that one can do better than adding an infinite series term by term if the goal is to get its sum to some specified numerical accuracy. This may appear as a paradox, but the truth is that several powerful techniques have been developed to that end since the arrival of the computer. The secret is to use hidden information in trailing digits of partial sums of the input series, to make assumptions on the form of the truncation error, and to subsequently eliminate that error by a suitably chosen algorithm. Success is judged by numerical experiments, and performance is the target.

A rather famous example for a problematic slowly convergent series is the Dirichlet series for the Riemann zeta function of argument 2,

$$\zeta(2) = \sum_{n=1}^{\infty} \frac{1}{n^2} \tag{1}$$

whose terms all have the same (positive) sign. It can be shown that a tenfold increase in the number of added terms improves the accuracy of the total sum only by a single decimal. When applying "usual" convergence acceleration methods like the epsilon algorithm [1] to *non-alternating* series, severe numerical instabilities are more likely the rule than the exception, and in general, more sophisticated algorithms have to be sought. We have found that the *combination* of two transformations leads to convincing numerical results in many applications. The two steps are: (i) a Van Wijngaarden transformation which transforms the nonalternating input series into an alternating series, and (ii) the acceleration of the Van Wijngaarden transformed series by a delta transformation. Details of the two transformations can be found in [2], and further developments will be published in [3]. Here, we are just going to state that the partial sums of the input, denoted s_n, are double-transformed to a series of transforms $\delta_n^{(0)}(1, \mathbf{S}_n)$ according to the

COMBINED NONLINEAR–CONDENSATION TRANSFORMATION (CNCT),

that is $s_n \to \delta_n^{(0)}(1, \mathbf{S}_n)$, where the $\delta_n^{(0)}(1, \mathbf{S}_n)$ exhibit much faster convergence than the input data s_n. The example in Table 1 concerns the evaluation of $\mathrm{Li}_3(0.99999)$ to a relative accuracy of 10^{-15} already in twelfth transformation order. This result can also be achieved by term-by-term summation of the defining series of Li_3 – in this case, however, about 100 million terms are required.

Table 1. Evaluation of $10^{-1}\,\mathrm{Li}_3(0.99999)$ with the CNC transformation [2].

n	$\delta_n^{(0)}(1, \mathbf{S}_0)$
0	0.133 331 333 415 539
1	0.120 474 532 168 000
2	0.120 176 326 936 846
3	0.120 204 748 497 388
4	0.120 204 079 128 106
5	0.120 204 045 387 208
6	0.120 204 045 378 284
7	0.120 204 045 434 802
8	0.120 204 045 438 553
9	0.120 204 045 438 726
10	0.120 204 045 438 733
11	0.120 204 045 438 733
12	0.120 204 045 438 733
exact	0.120 204 045 438 733

2 APPLICATIONS IN BIOPHYSICS

The theoretical description of biological processes is unthinkable today without extensive statistical analysis, and concurrently, fields like "bioinformatics" and "computational biology" are emerging. Several important mathematical functions needed in the theory of statistical distributions are represented by slowly convergent series, and their computation can benefit to a large extent from using the CNCT proposed here. Examples include the *discrete Zipf-related distributions* whose probability mass functions are represented by the terms of infinite series defining Riemann zeta, generalized zeta, and polylogarithm functions and whose total probability is calculated with these functions. These distributions are used in statistical analysis of biological sequences (of RNA, DNA and protein molecules) and occurence analysis of folds of proteins [3]. The generalized representation of these distributions was shown to be in the form of the Lerch distributional family [3]–[5], which requires calculation of Lerch's Φ transcendent. The Φ transcendent is given by the following power series,

$$\Phi(z, s, v) = \sum_{n=0}^{\infty} \frac{z^n}{(n+v)^s} \,. \tag{2}$$

For $|z| < 1$, $|z| \approx 1$, the power series is very slowly convergent. Of particular importance is the case of a real argument $x \equiv z$. In the region $x \approx 1$, we found that the application of the CNC transformation [2] leads to a significant acceleration of the convergence, whereas for $x \approx -1$, numerical problems can be solved by the direct application of the delta transformation [see Eq. (8.4-4) of [6]] to the defining series (2). The Riemann zeta, generalized zeta, and polylogarithm functions are special cases of Lerch's transcendent. Further applications of this special function include the quantile function of *continuous* S *distributions* [7]. Finally, the evaluation of several hypergeometric functions and related hypergeometric distributions can be significantly enhanced using the CNCT. Needless to say, a fast and accurate computation of these special functions is of crucial importance in calculating various basic properties of these distributions, including moments, cumulative distribution functions and quantiles, and parameter estimations.

3 APPLICATIONS IN THEORETICAL PHYSICS

We will briefly mention that various *long-standing problems in theoretical physics* have recently been solved using computational methods based on convergence acceleration techniques. Examples include quantum electrodynamic bound state calculations [8], which yield a theoretical description of the most accurate physical measurements today (in some cases, laser spectroscopy has reached a relative accuracy of 10^{-14} [9]). Therefore, the calculations are of importance for the test of fundamental quantum theories and for the determination of fundamental physical constants. Further applications include the evaluation of quantum corrections to Maxwell equations, which are given by the "quantum electrodynamic effective action" [10]. This object is representable by a slowly convergent series and is phenomenologically important in the description of various astrophysical processes.

We also report that it is possible, in combining analytic results obtained in [11] with numerical techniques based on the CNCT, to evaluate the so-called Bethe logarithm in hydrogen to essentially arbitrary precision. Specifically, we obtain – for the 4P state – the result

$$\ln k_0(4\mathrm{P}) = -0.041\,954\,894\,598\,085\,548\,671\,037(1) \tag{3}$$

which is 9 orders of magnitude more accurate than the latest and most precise calculation recorded so far in the literature [12].

4 APPLICATIONS IN MATHEMATICS

As far as mathematics is concerned, we will quote from [13]: "In April 1993, Enrico Au-Yeung, an undergraduate at the University of Waterloo, brought to the attention of [David Bailey's] colleague Jonathan Borwein the curious fact that

$$\sum_{k=1}^{\infty} \left(1 + \frac{1}{2} + \cdots + \frac{1}{k}\right)^2 k^{-2} \quad = \quad \frac{17\pi^4}{360}$$

based on a computation to 500,000 terms. Borwein's reaction was to compute the value of this constant to a higher level of precision in order to dispel this conjecture. Surprisingly, his computation to 30 digits affirmed it. [David Bailey] then computed this constant to 100 decimal digits, and the above equality was still affirmed."

Many formulas similar to (4) have subsequently been established by rigorous proof [14]. Using the CNCT, it is easy to calculate the sum (4) to 200 digits, based on multiprecision arithmetic [13] and a Linux personal computer, within a few hours. In calculating the specific case (4) to an accuracy of 200 decimals, which *a priori* requires the calculation of about 10^{205} terms of the series, we report that roughly 84 000 terms are sufficient when employing the CNCT. This corresponds to an acceleration of the convergence by roughly 200 orders of magnitude.

5 CONCLUSION

The CNCT has become useful in a wide variety of application areas which extend beyond the original scope of the transformation [8]. Details of the implementation of the algorithm, in the three languages C, Fortran and Mathematica [15] will be presented at the conference. Sample files will also be made available for internet download at [16]. We have recently investigated further potential applications of the algorithms described here, such as the evaluation of generalized hypergeometric functions which can be of exquisite practical importance, with rather promising results. The rather general applicability of the convergence accelaration methods makes them very attractive tools in scientific computing.

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[‡] Present address:
Universität Freiburg,
Theoretische Quantendynamik,
Hermann–Herder–Straße 3,
79104 Freiburg im Breisgau,
Germany,
jentschura@physik.uni-freiburg.de.

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[15] Certain commercial equipment, instruments, or materials are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

[16] home pages: *http://aksenov.freeshell.org/*, and *http://tqd1.physik.uni-freiburg.de/~ulj*.