An Admittedly Incomplete Introduction to the Topics Presented at the Conference "Approximation and Extrapolation of Convergent and Divergent Sequences and Series" CIRM Luminy: September 28, 2009 – October 2, 2009

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In the early 18th century, revolutionary changes took place in mathematics, and the foundations for the development of calculus were laid (see for example [1, Chapter 17]). Differential and integral calculus greatly extended the arsenal of mathematical techniques and also contributed substantially to the usefulness of mathematics in engineering and the sciences.

As I see it, the major achievement of this period was that mathematicians learned how to use *limiting processes* for the definition and also evaluation of mathematical quantities. For example, functions were expressed by power series, which are generalizations of polynomials, and integrals were introduced as generalizations of quadrature sums.

These were tremendous achievements. However, the incorporation of limiting processes into mathematics also caused serious problems. Limiting processes are unproblematic as long as they lead to (sufficiently simple) closed form expressions, but if we have to perform such a limit *numerically*, we often face enormous technical problems. There are many infinite series, whose convergence is so slow that the conventional process of adding up its terms successively is hopeless, and many integrals, whose integrands behave

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in such a pathological way that the straightforward application of a conventional quadrature rule does not accomplish anything substantial. Another class of problems occur if infinite series or integrals do not converge at all in the usual sense.

Already the founders of calculus were aware of these problems. Accordingly, numerical techniques for the acceleration of convergence or the summation of divergent series are almost as old as calculus itself. The first series transformation was apparently published already in 1730 by Stirling [2, 3], and in 1755 Euler [4] published the series transformation which now bears his name.

In rudimentary form, convergence acceleration methods are even older. They were already used in 1654 by Huygens and in 1674 by Seki Kowa, who both tried to obtain better approximations to π [5, pp. 90 - 91]. In a book by Liem, Lü, and Shih [6, p. *ix*] it is mentioned that extrapolation methods were already used by the Chinese mathematicians Liu Hui (A.D. 263) and Zhu Chongzhi (429 - 500) for obtaining better approximations to π, but no further details are given.

In the early days of calculus, problems with slow convergence or divergence were particularly severe due to the extremely limited computational resources. Since we now have access to powerful computers, it is tempting to believe that these techniques are less important than they used to be. However, many modern numerical techniques – for example iterative schemes, discretization methods, or perturbation techniques – produce results that are actually elements of a sequence since they depend on one or several parameters that govern the rate of convergence. In such a case, the application of sequence transformations is an obvious idea.

The available computing power tempts us to tackle even extremely challenging problems, which occasionally turn out to be beyond the reach of even the most powerful computers and which may also demonstrate the inadequacy of certain numerical techniques. The spectacular increase of computing power in the second half of the 20th century has not only created an enormous demand for powerful numerical techniques in general, but also for convergence acceleration and summation methods in special.

It makes sense to divide the the history of sequence transformations into a precomputational and a modern era. The modern era starts with two articles by Shanks [7] and Wynn [8], which were published in 1955 and 1956, respectively. Shanks introduced a powerful sequence transformation, and Wynn showed that not only this sequence transformation but also Padé approximants [9] can be computed effectively by means of his celebrated epsilon algorithm. Also in 1955, Romberg [10] published a seminal article which showed that extrapolation techniques can be extremely useful in the context of numerical quadrature.

It is probably no coincidence that these highly influential articles were published at a time when computers started to became generally available. After all, applied mathematics is driven by technology.

The articles by Shanks [7], Wynn [8], and Romberg [10] had a huge impact. Firstly, they showed that some challenging numerical problems can be handled successfully with the help of convergence acceleration and summation techniques. Secondly, they inspired many others to work on the development of new and hopefully even more powerful sequence transformations.

In 1971, Brezinski [11] showed that certain weaknesses and limitations of Wynn's epsilon algorithm can be overcome by modifying its recursive scheme, yielding the so-called theta algorithm. In 1973, Levin [12] introduced a new sequence transformation which utilizes the information contained in explicit estimates of the truncation error of the input sequence. Levin's idea was later extended in collaboration with and by Sidi (see for example [13, 14, 15]). Levin's idea inspired also many others, including myself [16] and Homeier [17]. For those interested in the historical development of sequence transformations, I can recommend two articles by Brezinski [18, 19].

Padé approximants can also be viewed to be a special class of sequence transformations since they transform the partial sums of a (formal) power series to a doubly indexed sequence of rational functions. They are named after Padé's thesis [9], which appeared in 1892, although they had been introduced already in the 18th century by Lambert and Lagrange, respectively (see for example [5, pp. 136 - 139] or [18, p. 311]).

Actually, Padé and his predecessors Lambert and Lagrange had the misfortune that the computational resources, which are necessary to make these approximants useful as computational tools, did not exist yet. Computing Padé approximants with paper and pencil is no fun. Consequently, Padé approximants used to be something that in principle could be done with power series, but nobody would seriously consider doing it. As we all know, this changed very much when computers became generally available.

The extensive research on sequence transformations in general and on Padé approximants in special is also reflected by a large number specialized monographs which had been published in recent years: I am aware of monographs by Baker [20], Baker and Graves-Morris [21], Brezinski [5, 22, 23, 24, 25], Brezinski and Redivo Zaglia [26], Bultheel [27], Cuyt [28], Delahaye [29], Gilewicz [30], Liem, Lü, and Shih [6], Sidi [31], Walz [32], and Wimp [33].

But even the most sophisticated mathematical theories have only little impact if those, who could apply these theories, cannot be reached. Specialized monographs are not necessarily the best medium to spread the gospel. Fortunately, there are now quite a few books that discuss sequence transformations and related topics as computational tools in various contexts. Examples are books by Baker [34], Bender and Orszag [35], Bornemann, Laurie, Wagon, and Waldvogel [36], Cuyt and Wuytack [37], Gil, Segura, and Temme [38], Marchuk and Shaidurov [39], Pozzi [40], and Press, Teukolsky, Vetterling, and Flannery [41]. Moreover, there is a recent review by Caliceti, Meyer-Hermann, Ribeca, Surzhykov, and Jentschura [42],

So far, sequence transformations and Padé approximants have been very popular in theoretical physics. I strongly suspect that this is largely due to the importance of divergent series in quantum physics. Already in 1952, Dyson [43] had argued that perturbation expansions in quantum electrodynamics should diverge factorially. Around 1970, Bender and Wu [44, 45, 46] showed that factorially divergent perturbation expansions occur also in nonrelativistic quantum mechanics. Later, it was found that factorially divergent perturbation expansions were actually the rule in quantum physics rather than the exception (see for example [47, Table 1], [48], or the articles reprinted in the book by Le Guillou and Zinn-Justin [49]).

Ultimately, this caused a renaissance of divergent series. Summation methods are essential to give divergent perturbation series in quantum physics any meaning beyond mere formal expansions and to extract numerical information from them. The most important summation techniques used by theoretical physicists are undoubtedly Borel summation [50] and Padé approximants [9], but Levin-type transformations have also become more popular in recent years (see for example [51, 52, 53, 54, 55] and references therein).

So far, sequence transformations and related techniques have mainly been employed in theoretical physics and related fields, but this is changing. For example, Belkić and Belkić have applied Padé approximants in cancer diagnostics (see for example [56, 57] and references therein). But this is not the only from the perspective of a scientist unconventional application of Padé approximants. For instance, González-Concepción and Pestano-Gabino [58] applied Padé approximants in economics,

Last, but not least let me emphasize that it is now generally accepted that extrapolation techniques are extremely useful in numerical quadrature. Numerous examples can be found in the recent book by Kythe and Schäferkotter [59].

From my personal perspective, it is highly satisfactory that the combination of nonlinear extrapolation techniques with quadrature rules for oscillatory integrals turned out to be extremely useful for the evaluation of the so-called molecular multicenter integrals of exponentially decaying functions. These complicated three- and six-dimensional integrals, which were the topic of my PhD thesis [60], constitute one of the oldest and most challenging mathematical and computational problems of electronic structure theory. Safouhi converted these integrals to Fourier-type integrals with the help of an analytical result from my PhD thesis [60, Eq. (7.1-6) on p. 160], which was later published as [61, Eq. (3.7)]. For the evaluation of the highly oscillatory Fourier-type integrals, Safouhi combined quadrature rules with suitable convergence acceleration techniques (see for example [62, 63, 64, 65] and references therein). This may well be the currently most promising approach for the evaluation of these complicated integrals. Things, which I could not do in my thesis, can now be done quite effectively with the help of extrapolation techniques.

Let me finish with another subjective remark. I believe that a close interaction between mathematicians, who predominantly work *on* sequence transformations and related topics, and scientists and engineers, who are mainly interested in working *with* sequence transformations, is of utmost importance. Interdisciplinary cross-fertilization is essential for further progress in this fascinating research topic.

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