The Birth of Numerical Analysis

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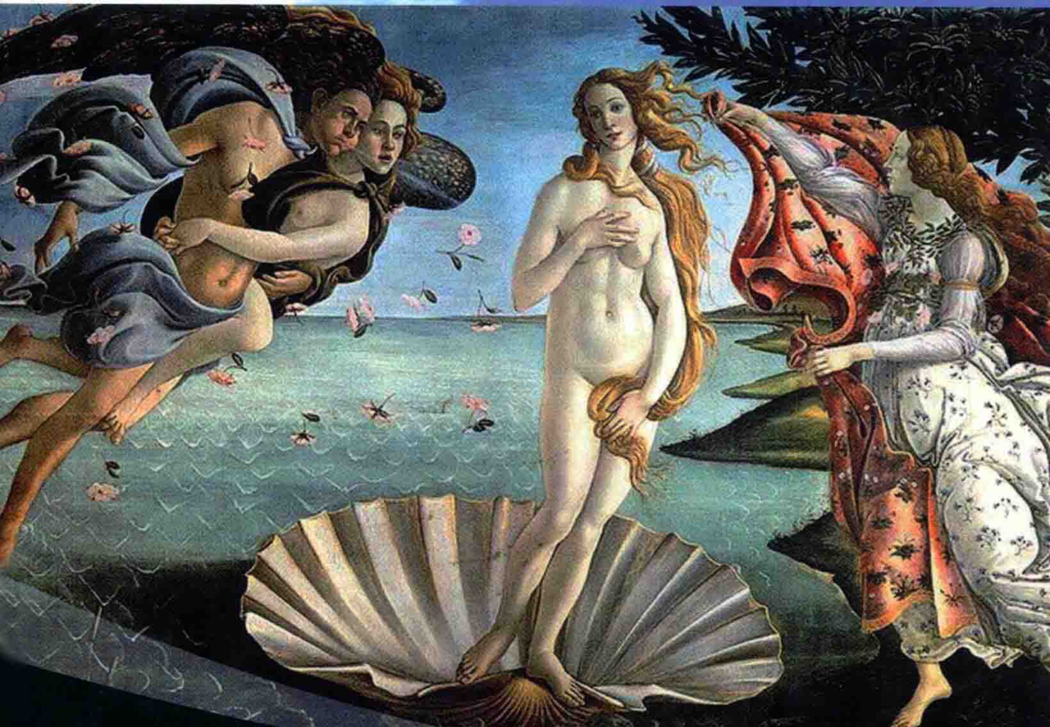
Adhemar Bultheel • Ronald Cools



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Katholieke Universiteit Leuven, Belgium

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THE BIRTH OF NUMERICAL ANALYSIS

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Preface

1 The limitations of computers

In Wikipedia, numerical analysis is described as that part of mathematics where algorithms for problems of continuous mathematics are studied (as opposed to discrete mathematics). This means that it is especially dealing with real and complex variables, the solution of differential equations and other comparable problems that feature in physics and engineering. A real number has in principle an infinite number of digits, but on a digital computer, only a finite number of bits is reserved to store a (real) number. This memory restriction implies that only rounded, approximating values of only finitely many real numbers can be stored. The naive idea of the early days of digital computers was that they would not make the same "stupid errors" that human computers sometimes made, like transcription errors, reading errors, wrong signs, etc. This euphoria was however soon tempered when it was realized that computers in fact make errors in practically every calculation. Small errors indeed, but nevertheless a lot of errors. And all these small errors can accumulate and grow like a virus through the many elementary computations made which could eventually give a result that is quite different from the exact one.

2 A birthday?

A careful analysis of this propagation of errors when solving a linear system of equations was first published in a paper by John von Neumann and Herman Goldstine: *Numerical inverting of matrices of high order*, published in the November issue of the *Bulletin of the American Mathematical Society* in 1947. Because this was the first time that such an analysis was made, this paper is sometimes considered to be the start of modern numerical analysis. Of course numerical calculations were done long before that paper and problems from physics and engineering had been solved earlier, but the scale and the complexity of the computations increased drastically with the introduction of digital computers. The "large systems" to which the title of the paper refers, would not be called "large" at all by current standards. It is claimed in the paper that "serious problems can occur" if one wants to solve systems of more than ten equations. In a subsequent footnote, it is suggested that it would probably be possible in the future to solve systems of a hundred equations. If we know that the PageRank of Google can be computed by manipulating systems of approximately ten billion equations, then it should be clear we have come a long distance.

3 Sixty years young "back to the roots of the future"

If the publication of the von Neumann-Goldstine paper is indeed the start of numerical analysis, then November 2007 would be the moment that numerical analysis can celebrate its sixtieth birthday. This inspired the scientific research network *Advanced Numerical Methods for Mathematical Modeling*, a consortium of numerical analysis groups in Flanders, to organize a two-day symposium at the Department of Computer Science of the K.U.Leuven (Belgium) entitled *"The birth of numerical analysis"*. The idea of this symposium was to invite a number of speakers who were already active numerical analysts around the middle of the twentieth century or shortly after and hence were co-founders of the modern discipline. They came to witness about their experience during the early days and/or how their respective subdomains have evolved. Back to the roots is an important general cultural paradigm, and it is none the less true for numerical analysis. To build a sound future, one must have a thorough knowledge of the foundations. Eleven speakers came to Leuven on October 29-30, 2007 for this event to tell their personal story of the past and/or give their personal vision of the future. In the rest of this preface we give a short summary of their lectures. Most of them have also contributed to these proceedings.

4 Extrapolation

The start of the symposium was inspired by extrapolation. In many numerical methods, a sequence of successive approximations is constructed that hopefully converges to the desired solution. If it is expensive to compute a new approximation, it might be interesting to recombine a number of the last elements in the sequence to get a new approximation. This is called extrapolation (to the limit). In the talk of *Claude Brezinski*, a survey was given of the development of several extrapolation methods. For example for the computation of π, Christiaan Huygens used in the seventeenth century an extrapolation technique that was only rediscovered by Richardson in 1910, whose name has been attached to the method. Another extrapolation method was described by Werner Romberg in 1955. He tried to improve on the speed of convergence of approximations to an integral generated by the trapezium rule. This method is now called Romberg integration. After the introduction of digital computers, the improvements, generalizations, and variations of extrapolation techniques were numerous: Aitken, Steffensen, Takakazu, Shanks, Wynn, QD and epsilon algorithms are certainly familiar to most numerical analysts. Read more about this in Brezinski's contribution of this book.

> Claude Brezinski (°1941) is emeritus professor at the University of Lille and is active on many related subjects among which extrapolation methods but also Padé approximation, continued fractions, orthogonal polynomials, numerical linear algebra and nonlinear equations. He has always shown a keen interest in the history of science, about which he has several books published.

The talk of *James Lyness* connected neatly with the previous talk. Romberg integration for one-dimensional integration also got applications in more-dimensional integration, but the first applications only came in 1975 for integrals over a simplex and integrands with a singularity. Nowadays this has become an elegant theory for integration of functions with an algebraic or logarithmic singularity in some vertices of a polyhedral domain of integration. The integration relies on three elements. Suppose we have a sequence of quadrature formulas $Q^{[m]}\{f\}$ that converge to the exact integral: $I\{f\} = Q^{[\infty]}\{f\}$. First one has to write an asymptotic expansion of the quadrature around $m = \infty$. For example $Q^{[m]}\{f\} = B_0 + B_1/m^2 + B_4/m^4 + \cdots + B_{2p}/m^{2p} + R_{2p}(m)$ with $B_0 = I\{f\}$. This is just an example and the form of the expansion should be designed in function of the singularity of the integrand. Next, this is evaluated for say n different values of m, which results in a system of n linear equations that is eventually solved for the B_k, in particular $B_0 = I\{f\}$. The moral of the story is that for further development of multidimensional extrapolation quadrature one only needs three simple elements: a routine to evaluate the integrand, a routine implementing the quadrature rule, and a solver for a linear system. Of course the most difficult and most creative part is to find the appropriate expansion.

The contribution of Lyness is included in these proceedings.

James Lyness (°1932) is employed at the Argonne National Laboratory and the University of New South Wales. His first publications appeared mainly in physics journals, but since he published his first paper on N-dimensional integration (co-authored by D. Mustard and J.M. Blatt) in *The Computer Journal* in 1963, he has been a leading authority in this domain with worldwide recognition.

5 Functional equations

The afternoon of the first day was devoted to functional equations.

From an historical point of view, we could say that the method of Euler for the solution of ordinary differential equations (1768) is the seed from which all the other methods were deduced. That is how it was presented in the lecture of *Gerhard Wanner*. Runge, Heun and Kutta published their methods around 1900. These were based on a Taylor series expansion of the solution and the idea was to approximate it in the best possible way. This means that for a small step h, the difference between the true and the approximating solutions was $O(h^p)$ with order p as high as possible. Such an approach quickly leads to very complicated systems of equations defining the parameters of the method. Therefore in the sixties and seventies of the previous century, much effort was put in a systematic treatment by, e.g., Butcher, Hairer and Wanner.

On the other hand, multistep methods are among the offspring of techniques by Adams and Bashforth which date back to 1885. These predict the next value of the solution using not only the last computed point, such as Runge-Kutta methods do, but they use several of the previously computed points to make the prediction. Dahlquist published in 1956 the generalized linear multistep methods. Important efforts have been made to improve the step control and the stability.

> Gerhard Wanner (°1942) is professor at the University of Genève and ex-president of the Suisse Mathematical Society. He wrote together with Hairer several books on analysis and differential equations. The historical aspects always played an important role. He has had scientific contacts at all "levels" from 2 meter below sea level (the Runge-Kutta symposium at the CWI in Amsterdam on the occasion of 100 years of Runge-Kutta methods in 1995) to the top of the Mont Blanc at 4807 meters above sea level where he hiked together with Hairer.

The further development was picked up in the talk by *Rolf Jeltsch*. His main topic was the evolution of the concept of stability when solving stiff differential equations.

Stiff differential equations form a problem for numerical solution methods because the dynamics of the solution have components at quite different scales. Researchers wanted to design methods that computed numerically stable (bounded) solutions when the theoretical solution was supposed to be stable. Dahlquist proved in 1963 his well known second barrier for multistep methods. It stated that there was not an A-stable method of order higher than two. The A stands for absolute, which means that the numerical method computed a stable solution, whatever the step size is. This started a quest for other types of methods and gave rise to a whole alphabet of weaker types of stability.

> Rolf Jeltsch (°1945) is professor at the ETH Zürich. He is a former president of the EMS (1999-2002) and of the Suisse Mathematical Society (2002-2003). Since 2005 he is president of the "Gesellschaft für Angewandte Mathematik und Mechanik" (GAMM). In the nineteen seventies his main research topic was ordinary differential equations. Since the nineteen eighties, he focussed more on hyperbolic partial differential equations and large scale computations in engineering applications.

Unfortunately, the contributions by Wanner and Jeltsch could not be included in these proceedings but the editors were happy to find a valuable replacement to cover the area of differential equations. *John Butcher* provided a text in which he reports on the contribution of New Zealanders, which includes his own, to numerical analysis in general and differential equations in particular. So he links up the European and New Zealand numerical scene. His personal reminiscences bring about a broader historical perspective.

> John Butcher (°1933) is professor emeritus at the Department of Mathematics, of the University of Auckland. His main interests are in the numerical solution methods for ordinary differential equations. He is considered to be the world's leading specialist on Runge-Kutta methods. His 1987 book on the numerical solution of ordinary differential equations and their subsequent editions of 2003 and 2008, are considered the best reference work on this subject.

Herbert Keller was the dean of the company. He replaced Philip Davis, who first agreed to attend but eventually was not able to come to the meeting. The message of Keller was that singularities have always played an important role in numerical computations and that they were not always given the attention they deserve. This starts with such a simple thing as dividing by zero (or by something "almost zero"). This is obviously a fundamental issue. In Gaussian elimination for solving a linear system of equations, dividing by a small diagonal element may completely destroy the accuracy of the algorithm. But, it is as important to take care of a singularity of an integrand when designing good numerical quadrature formulas. This was already shown in the talk by Lyness. Another example is encountered when solving nonlinear equations where the Jacobian evolves during the iteration towards a matrix that is (almost) singular. This kind of difficulties certainly appears in more complex large scale problems connected with differential or integral equations, dynamical systems etc.

Herb Keller was in excellent shape during the symposium and full of travel plans. However, few months after the symposium, we received the sad news that Keller had passed away on January 26, 2008. So there is no contribution by him about his talk. Hinke Osinga, who had an interview with Keller published in the DSWeb Magazine, was kind enough to slightly adapt her text and this is included instead.

Herbert Keller (°1925 – †2008) was emeritus professor at the California Institute of Technology. Together with E. Isaacson, he is the author of the legendary book "Analysis of Numerical Methods" that was published in 1966 by J. Wiley. His scientific contributions mainly dealt with boundary value problems and methods for the solution of bifurcation problems.

The first day was concluded by the lecture of *Kendall Atkinson* who spoke about his personal vision on the evolution in research related to the solution of integral equations. He emphasized the use of functional analysis and operator theory for the analysis of numerical methods to solve this kind of equations. The origin points to a paper by Kantorovich "Functional analysis and applied mathematics" that appeared in Russian in 1948. It deals among other things with the solution of Fredholm integral equations of the second kind. Atkinson summarizes the most important methods and the results that were obtained: degenerate kernel approximation techniques in which the kernel is written as $K(s,t) = \sum_i \alpha_i(s)\beta_i(t)$, projection methods (the well known Galerkin and collocation methods where the solution is written as a linear combination of basis functions with coefficients that are fixed by interpolation or by orthogonality conditions), and the Nyström method that is based on numerical integration. The details of his lecture can be found in these proceedings.

Kendall Atkinson (°1940) is emeritus professor at the University of Iowa. He is an authority in the domain of integral equations. His research encompasses radiosity equations from computer graphics and multivariate approximation, interpolation and quadrature. He wrote several books on numerical analysis and integral equations.

6 The importance of software and the influence of hardware

The first lecture of the second day was given by *Brian Ford*. He sketched the start and the development of the NAG (Numerical Algorithms Group) software library. That library was the first collection of general routines that were not just focussing on one particular kind of numerical problem or on one particular application area. Also new was that it came out of the joint effort of several researchers coming from different groups. Ford started up his library in 1967, stimulated by his contacts with J. Wilkinson and L. Fox. Being generally applicable, well tested, and with good documentation it was an immediate success. The official start of the Algol and Fortran versions of the NAG library is May 13, 1970. The algorithms are chosen on the basis of stability, robustness, accuracy, adaptability and speed (the order is important). Ford then tells about the further development and the choices that had to be made while further expanding the library and how this required an interplay between numerical analysts and software designers. He concludes his talk with an appeal to young researchers to work on the challenge put forward by the new computer architectures where multicore hardware requires a completely new implementation of the numerical methods if one wants to optimally exploit the computing capacity to cut down on computer time and hence to solve larger problems.

The contribution of B. Ford is included in these proceedings. More on the (r)evolution concerning hardware and its influence on the design and implementation of numerical software can be found in the next contribution by J. Dongarra.

> Brian Ford (°1940) is the founder of the NAG company and was director until his retirement in 2004. He received a honorary doctorate at the University of Bath and was given a OBE (Officer of British Empire) for his achievements. Under his leadership, NAG has developed into a respected company for the production of portable and robust software for numerical computations.

The conclusion of B. Ford was indeed the main theme in the lecture of *Jack Dongarra*. In his lecture he describes how, since about 1940, the development of numerical software, the hardware, and the informatics tools go hand in hand. Early software was developed on scalar architectures (EISPACK, LINPACK, BLAS '70) then came vector processors ('70-'80) and parallel algorithms, MIMD machines (ScaLAPACK '90), and later SMP, CMP, DMP, etc. The multicore processors are now a reality and a (r)evolution is emerging because we will have to deal with multicore architecture that will have hundreds and maybe thousands of cores. Using all this potential power in an efficient way by keeping all these processors busy, will require a total re-design of numerical software.

A short version of the lecture, concentrating on a shorter time-span, has been included in these proceedings.

Jack Dongarra (°1950) is professor at the University of Tennessee where he is the leader of the "Innovative Computing Laboratory". He is specialized in linear algebra software and more generally numerical software on parallel computers and other advanced architectures. In 2004 he received the "IEEE Sid Fernbach Award" for his work in HPC (High Performance Computing). He collaborated on the development of all the important software packages: EISPACK, LINPACK, BLAS, LAPACK, ScaLAPACK, etc.

7 Approximation and optimization

More software in the lecture of *Robert Plemmons*. The thread through his lecture is formed by nonnegativity conditions when solving all kinds of numerical problems. First a survey is given of historical methods for the solution of nonnegative least squares problem. There one wants to solve a linear least squares problem where the unknowns are all nonnegative. Also the factorization of two nonnegative matrices (NMF) was discussed. The latter is closely connected with data-analysis. Other techniques used here are SVD (singular value decomposition) and PCA (principal component analysis). These however do not take the nonnegativity into account. Around the nineteen nineties ICA (independent component analysis) was introduced for NMF. This can also be formulated as BSS (blind source separation). In that kind of application, a mixture of several sources is observed and the problem is to identify the separate sources. In more recent research, one tries to generalize NMF by replacing the matrices by tensors. There are many applications: filter out background noise from an acoustic signal, filtering of e-mails, data mining, detect sources of environment pollution, space research SOI (space object identification) etc.

Read more about this in the contribution by Chen and Plemmons in these proceedings.

Robert J. Plemmons (°1938) is Z. Smith Reynolds professor at the Wake Forest University, NC. His current research includes computational mathematics with applications in signal and image processing. For example, images that are out of focus are corrected, or atmospheric disturbances are removed. He published more than 150 papers and three books about this subject.

Michael Powell gave a survey of the successive variants of quasi-Newton methods or methods of variable metric for unconstrained nonlinear optimization. He talked about his contribution to their evolution of the prototypes that were designed in 1959. These methods were a considerable improvement over previous methods that were popular before that time which were dominated by conjugate gradients, pure Newton, and direct search methods. In these improved methods, an estimate for the matrix of second derivatives is updated so that it does not have to be recomputed in every iteration step. These methods converge fast and the underlying theory is quite different from the corresponding theory for a pure Newton method. Mike Powell then evoked methods derived from the previous ones that are important in view of methods for optimization problems with constraints. Further methods discussed are derivative free methods, and the proliferation of other types like simulated annealing, genetic algorithms etc.

A summary of this presentation can be found in these proceedings.

Michael J.D. Powell (°1936) is professor at Cambridge University. He has been active in many domains. His name is for example attached to the DFP (Davidon-Fletcher-Powell) method (a quasi-Newton method for optimization), and a method with his name that is a variant of the Marquardt method for nonlinear least squares problems. But he is also well known for his work in approximation theory. The Powell-Sabin splines are still an active research area in connection with subdivision schemes for the hierarchical representation of geometric objects or in the solution of partial differential equations.

8 And some history

The closing lecture of the symposium was given by *Alistair Watson.* With some personal touch, he sketched the early evolution of numerical analysis in Scotland. In a broader sense, numerical analysis has existed for centuries of course. If you restrict it to numerical analysis as it was influenced by digital computers, then 1947 is a good choice to call that the start. But thinking of the more abstract connection between numerics and computers, then one should probably go back to 1913 when papers by Turing were published. That is where Watson starts his account of the history. More concretely, in Scotland, the start is associated with the work of Whittaker and later Aitken who were appointed in Edinburgh. In the "Mathematical Laboratory", founded in 1946, computations were done by means of pocket calculators. It was only in 1961 that this was coined to be a "Numerical Analysis" course. In that year Aitken claimed to have no need for a digital computer. It arrived anyway in 1963. Then things start to move quickly. More numerical centers came into existence in St Andrews and later in Dundee. The University of Dundee became only independent of St Andrews in 1967 and soon the gravity center of numerical analysis had moved to Dundee. From 1971 until 2007, the biennial conference on numerical analysis was held in Dundee. In the most recent years, the University of Strathclyde (Glasgow) seems to be the new attraction pole for numerical analysis in Scotland.

A longer write-up of this historical evolution is included in these proceedings.

The focus of the work of Alistair Watson (°1942) is numerical approximation and related matters. This can be theoretical aspects, but also elements from optimization and linear algebra. He is FRSE (Fellow of the Royal Society of Edinburgh) and he is probably best known by many for his involvement in the organization of the Dundee conferences on numerical analysis.

9 And there is more

Of the eleven lecturers at the symposium, the youngest was 57 and the oldest 82, with an average just over 68. All of them showed a lot of enthusiasm and made clear that whatever the exact age of numerical analysis, be it sixty years or a hundred years or even centuries, there still remains a lot to be done and the challenges of today are greater than ever.

Of course we would have liked to have invited many more people to lecture and cover more subjects at the symposium, but time and budget was finite. Some important people who had planned to come, finally decided for diverse reasons to decline. One of these was *Gene Golub* (°1932 – †2007), the undisputed godfather of numerical linear algebra, who, sad to say, passed away just after the symposium on November 19, 2007. Another name we would have placed on our list as a speaker for his contributions to numerical integration would have been *Philip Rabinowitz* (°1926 – †2006) had he still be among us. We are fortunate to have obtained permission of the American Mathematical Society to reprint an obituary with reminiscences of Phil Davis and Aviezri Fraenkel that was first published in the Notices of the AMS in December 2007.

Phil Davis also wrote up some personal reminiscences of what it was like in the very early days, when numerical analysis was just starting in the years before and during WW-II.

> Philip Davis (°1923), currently emeritus professor at Brown University. He is well known for his work in numerical analysis and approximation theory, but with his many columns, and books, he also contributed a lot to the history and philosophy of mathematics. His books on quadrature (together with Ph. Rabinowitz) and on interpolation and approximation are classics. He also collaborated on the Abramowitz-Stegun project *Handbook of Mathematical Functions*. He started his career as a researcher in the Air Force in WW-II, and joined the National Bureau of Standards before going to Brown.

Finally, we found *Robert Piessens* kind enough to write another contribution for this book. His approach is again historical and sketches first the work of Chebyshev about linkage instruments, a mechanical tool to transform a rotation into a straight line. This is how Chebyshev polynomials came about. He continues by illustrating how the use of Chebyshev polynomials has influenced the research of his group at K.U.Leuven, since it turned out to be a powerful tool in developing methods for the numerical solution of several problems encompassing inversion of the Laplace transform, the computation of integral transforms, solution of integral equations and evaluation of integrals with a singularity. The latter resulted in the development of the QUADPACK package for numerical integration.

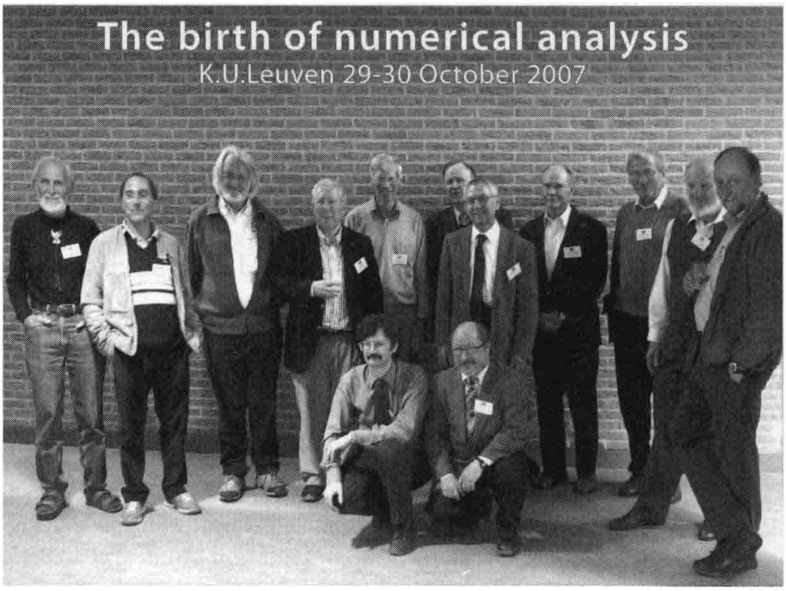
> Robert Piessens (°1942) is emeritus professor at the Department of Computer Science at the K.U.Leuven, Belgium. He was among the first professors who started up the department. His PhD was about the numerical

inversion of the Laplace transform. He is one of the developers of the QUADPACK package which has been a standard package for automatic numerical integration in one variable. Originally written in Fortran 77, it has been re-implemented in different environments. It is available via netlib, several of its routines have been re-coded and are integrated in Octave and Matlab, the Gnu Scientific Library (GSL) has a C-version, etc.

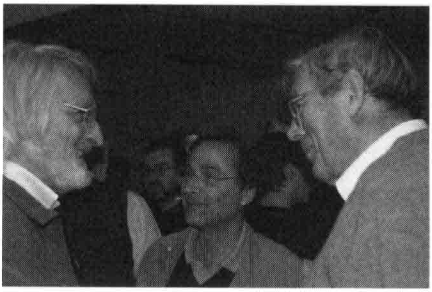
10 Acknowledgements

The symposium was sponsored by the FWO-Vlaanderen and the FNRS, the regional science foundations of Belgium. We greatefully acknowledge their support.

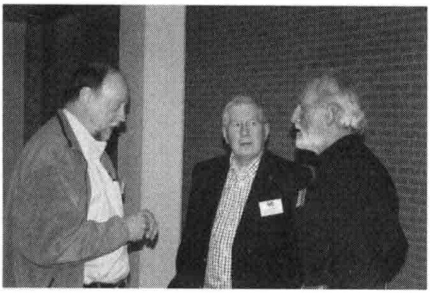
Leuven, March 2009 Adhemar Bultheel and Ronald Cools



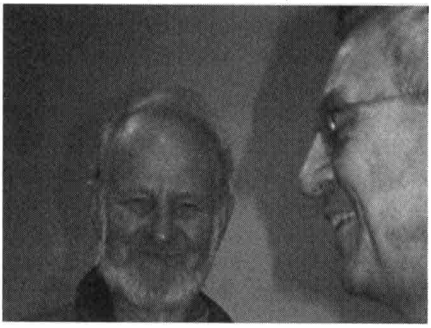
From left to right:
H. Keller, C. Brezinski, G. Wanner, B. Ford, A. Watson, K. Atkinson, R. Jeltsch, R. Plemmons, M. Powell, J. Lyness, J. Dongarra.
In front: the organizers:
R. Cools and A. Bultheel



G. Wanner, C. Brezinski, M. Powell

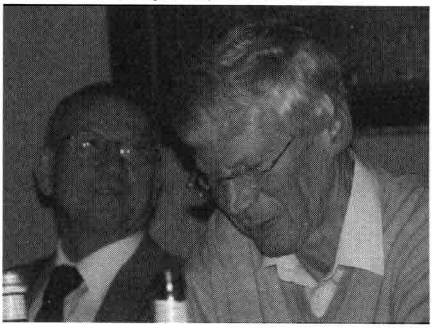


J. Dongarra, B. Ford, H. Keller



J. Lyness, R. Jeltsch

B. Plemmons, M. Powell



R. Jeltsch, A. Watson

B. Ford, K. Atkinson

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Some pioneers of extrapolation methods

Claude Brezinski

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Abstract. There are two extrapolation methods methods which are described in almost all numerical analysis books: Richardson's extrapolation method (which forms the basic ingredient for Romberg's method), and Aitken's Δ^2 process. In this paper, we consider the historical roots of these two procedures (in fact, the computation of π) with an emphasis on the pioneers of this domain of numerical analysis. Finally, we will discuss some more recent developments and applications.

Richardson's extrapolation method and Aitken's Δ^2 process are certainly the most well known methods for the acceleration of a slowly converging sequence. Both are based on the idea of extrapolation, and they have their historical roots in the computation of π.

We will first explain what extrapolation methods are, and how they lead to sequence transformations for accelerating the convergence. Then, we will present the history of Richardson's extrapolation method, of Romberg's method, and of Aitken's Δ^2 process, with an emphasis on the lives and the works of the pioneers of these topics.

The study of extrapolation methods and convergence acceleration algorithms now forms an important domain of numerical analysis having many applications; see [15, 24, 71, 77, 78, 80]. More details about its mathematical developments and its history could be found in [11, 13, 26, 34].

1 Interpolation, extrapolation, sequence transformations

Assume that the values of a function f are known at k distinct points x_i, that is

$$y_i = f(x_i), \quad i = 0, \ldots, k-1.$$

Choose a function F_k depending on k parameters $a_0, \ldots, a_{k-1}$, and belonging to some class of functions $\mathcal{F}_k$ (for example polynomials of degree $k-1$).

What is interpolation? Compute $a_0^e, \ldots, a_{k-1}^e$ solution of the system of equations (the meaning of the superscript $.^e$ will appear below)

$$F_k(a_0^e, \ldots, a_{k-1}^e, x_i) = y_i, \quad i = 0, \ldots, k-1. \tag{1.1}$$