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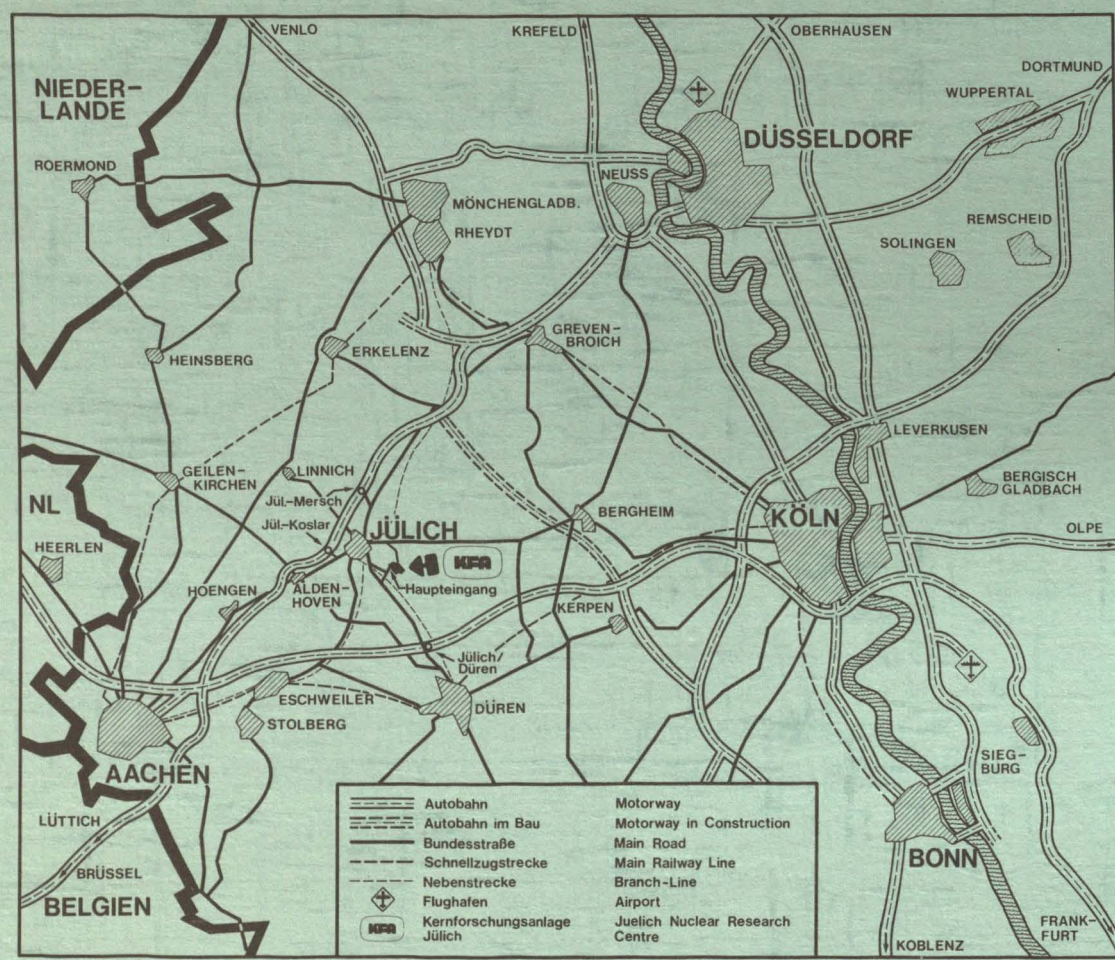

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Contents

Summary

The accuracy of numerical inversion methods for Laplace transforms depends as well on the algorithm as on the given Laplace transform. An algorithm may lead to excellent results for a certain problem and fail completely for another one.

In this report the theory and the application of a new inversion procedure (see [7]) are described. The procedure is based on a Fourier series expansion and achieves, compared with other inversion methods, a very high accuracy with only a few function evaluations of the Laplace transform. This is due to some efficient algorithms reducing the discretization and truncation error of the Fourier series approximation and an algorithm determining the optimal parameters of the procedure. Furthermore, the variety of algorithms offered by the new inversion procedure allows its successful application in a very big range of applications.

Several typical examples were selected to demonstrate the mentioned properties and to show the user how to take advantage of certain possibilities such as to calculate approximately the total error, to avoid misleading results by using available 'control digits', or to find, for a given problem, the most efficient combination of the different algorithms.

The procedure is implemented as a FORTRAN subroutine. This subroutine, called LAPIN, can also be used as a "black box": the only input parameters the user has to define in that case are the t-values for which $f(t) = L^{-2}[F(s)]$ shall be computed, and of course the Laplace transform $F(s)$. The available algorithms are selected automatically.

1. Introduction

The significance of numerical Laplace inversion is obvious from the big range of applications. Well known in engineering, Laplace transformation methods are also used in order to solve differential and integral equations and to assist when other numerical methods are applied (see [10]).

A number of numerical inversion methods has been developed during the last few years. In chapter 2 of this report we describe inversion procedures (see [7]) based on Fourier series expansions. Many tests (see [4], [5], [8], [2], [1]) have shown that methods using Fourier series approximations are superior to others in accuracy and simplicity.

Fourier series were first used by Dubner and Abate [4] in 1968 for the numerical inversion of Laplace transforms. Durbin [5] improved the method in 1973.

Other authors (Simon et al. [8] in 1972, Veillon [9] in 1972 and Crump [2] in 1976) used different acceleration methods in order to speed up the convergence of the Fourier series derived in [4] and [5]. Some of these methods at times achieve a considerable reduction of the truncation error. However, they fail in other cases and their efficiency heavily depends on the choice of the parameters of the methods of Durbin or Dubner and Abate; and the choice of these parameters was somewhat arbitrary.

The biggest disadvantage of the above mentioned methods is the dependence of the discretization and truncation errors

on the free parameters: by a suitable choice of these parameters the discretization error becomes arbitrarily small, but at the same time the truncation error grows to infinity, and vice versa. A first step in surmounting this problem was taken in [1], 1977 (see part 2.2) , where the so-called "Korrektur"-method was presented. It allows a remarkable reduction of the discretization error without increasing the truncation error.

Nevertheless the accuracy of the "Korrektur"-method also depends on a 'good' choice of the free parameters. The procedure introduced in part 2.4 gets closer to the solution of the problem. It allows the approximate computation of optimal parameters for all above mentioned methods (for the definition of "optimal" see part 2.4).

Part 2.3 describes a new method for the acceleration of convergence of the Fourier series. It is applicable if the finite series for the approximation of the inversion integral does not alternate (see part 2.3). In this case all other tested acceleration methods failed.

In parts 2.1 and 2.3,those of the above mentioned inversion and acceleration methods that were found to be optimal by numerical tests as well as by the derived error estimates are summarized.

A new algorithm for the numerical Laplace inversion, taking into consideration the procedures described in part 2, is

implemented as a FORTRAN subroutine [1] [7].

This subroutine, called LAPIN, can be used as a "black box": the only input parameters are the t-values for which $f(t) = L^{-1}[F(s)]$ shall be computed and of course the Laplace transform $F(s)$. On the other hand - for a concrete problem - the user can make an optimal choice of all free parameters in order to have the most efficient combination of the algorithms contained in the subroutine.

In chapter 3 we show by several typical examples how these parameters have to be chosen to get high accuracy with only a few function evaluations of the Laplace transform.
The difficulties arising with the application of acceleration methods are discussed and hints are given to overcome them.

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[1] See chapter 3, subroutine LAPIN (LAPlace INversion).

2. The numerical inversion of Laplace transforms by Fourier series expansions

2.1 The method of Durbin

The Laplace transform of a real function $f: \mathbb{R} \to \mathbb{R}$ with $f(t) = o$ for $t<o$ and its inversion formula are defined as

$$F(s) = L[f(t)] = \int_0^\infty e^{-st} f(t)\, dt\,, \tag{1}$$

$$f(t) = L^{-1}[F(s)] = \frac{1}{2\pi i} \int_{v-i\infty}^{v+i\infty} e^{st} F(s)\, ds \tag{2}$$

with $s = v + iw$; $v,w \in \mathbb{R}$.

$v \in \mathbb{R}$ is arbitrary, but greater than the real parts of all the singularities of $F(s)$. The integrals in (1) and (2) exist for $Re(s) > a \in \mathbb{R}$ if

(a) f is locally integrable,

(b) there exist a $t_o \geq o$ and k , $a \in \mathbb{R}$ such that $|f(t)| \leq ke^{at}$ for all $t \geq t_o$, (3)

(c) for all $t \in (o,\infty)$ there is a neighbourhood in which f is of bounded variation.

In the following we always assume that f fulfils the conditions (3) and in addition that there are no singularities of $F(s)$ to the right of the origin. Therefore (1) and (2) are defined for all $v>o$. The possibility to choose $v>o$ arbitrarily, is the basis of the methods of Dubner/Abate and Durbin. The latter is now described.

Using the inversion formula (see [5])

$$f(t) = \frac{e^{vt}}{\pi} \int_o^\infty [Re\{F(s)\} \cos(wt) - Im\{F(s)\} \sin(wt)]\, dw\,, \tag{4}$$

which is equivalent to (2), and a Fourier series expansion of $h(t) = e^{-vt} f(t)$ in the interval $[o,2T]$, Durbin derived the approximation formula

$$f(t) = \frac{e^{vt}}{T} \left[-\frac{1}{2} \mathrm{Re}\{F(v)\} + \sum_{k=o}^{\infty} \mathrm{Re}\{F(v + i\frac{k\pi}{T})\} \cos \frac{k\pi}{T} t \right. \\ \left. - \sum_{k=o}^{\infty} \mathrm{Im}\{F(v + i \frac{k\pi}{T})\} \sin \frac{k\pi}{T} t\right] - F1(v,t,T) \tag{5}$$

for $o < t < 2T$.

$F1(v,t,T)$ is the discretization error, given by

$$F1(v,t,T) = \sum_{k=1}^{\infty} e^{-2vkT} f(2kT + t) . \tag{6}$$

Since there are no singularities of $F(s)$ in the right halfplane we have[2] a $c > o$, $m \geq o$ and a $t_o \geq o$, such that

$$|f(t)| \leq ct^m \quad \text{for all} \quad t \geq t_o . \tag{7}$$

From (6) and (7) the following estimates for the discretization error can be deduced (see [5]):

a) $m = o$

$$|F1(v,t,T)| \leq \frac{c}{e^{2vT} - 1} , \tag{8}$$

b) $m > o$

$$|F1(v,t,T)| \leq K(2T)^m e^{-2vT} \left(\frac{\alpha_1}{2vT} + \ldots + \frac{\alpha_{m+1}}{(2vT)^{m+1}}\right) \tag{9}$$

where $K, \alpha_1, \ldots, \alpha_{m+1} \in \mathbb{R}$.

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[2] See Doetsch [3], Bd. 1

These estimates show that the discretization error can be made arbitrarily small by choosing v sufficiently large.
As the infinite series in (5) can only be summed up to a finite number N of terms, there also occurs a truncation error given by

$$FA(N,v,t,T) = \frac{e^{vt}}{T}\left[\sum_{k=N+1}^{\infty}\{Re\{F(v+\frac{ik\pi}{T})\}\cos\frac{k\pi}{T}t - Im\{F(v+\frac{ik\pi}{T})\}\sin\frac{k\pi}{T}t\}\right] . \tag{10}$$

Hence the approximate value for $f(t)$ is

$$f_N(t) = \frac{e^{vt}}{T}\left[-\frac{1}{2}Re\{F(v)\} + \sum_{k=o}^{N}\{Re\{F(v+\frac{ik\pi}{T})\}\cos\frac{k\pi t}{T} - Im\{F(v+\frac{ik\pi}{T})\}\sin\frac{k\pi t}{T}\}\right] . \tag{11}$$

2.2 The "Korrektur"-method

It is obvious from (8) and (9) that the discretization error can be made arbitrarily small if the product vT is sufficiently large.

Unfortunately, the truncation error (1o) may diverge for large values of vT .

The "Korrektur"-method allows a reduction of the discretization error without enlarging the truncation error.
With (11) equation (5) can be written in the form

$$f(t) = f_\infty(t) - F1(v,t,T) \quad . \tag{12}$$

The "Korrektur"-method uses the approximation formula

$$f(t) = f_\infty(t) - e^{-2vT} f_\infty(2T+t) - F2(v,t,T) \quad . \tag{13}$$

As stated in the theorem below, the discretization error $F2(v,t,T)$ is much smaller than $F1(v,t,T)$.

Taking into consideration the truncation error (1o), we find that the approximate value for $f(t)$, using the "Korrektur"-method (13), is given by

$$f_{NK}(t) = f_N(t) - e^{-2vT} f_{N_o}(2T + t) \quad . \tag{14}$$

It should be mentioned that the truncation error of the "Korrektur"-term $e^{-2vT} f_\infty(2T + t)$, is much smaller than $FA(N,v,t,T)$ if $N=N_o$. We can therefore choose $N_o < N$ [3)],

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3) see part 3.2 .

which means that only a few additional function evaluations of $F(s)$ are necessary to achieve a considerable reduction of the discretization error. This error reduction is pointed out in the following theorem.

Theorem 2.1 : Suppose f is a real function with $f(t) = o$ for $t < o$ that possesses the properties (3) and $F(s) = L[f(t)]$ its Laplace transform that has no singularities to the right of the origin, and suppose the "Korrektur"-formula (13) is used for the numerical inversion of $F(s)$, then

$$\text{a)} \quad |F2(v,t,T)| \leq \frac{2c}{e^{2vT}(e^{2vT} - 1)} \tag{15}$$

if $m = o$,

$$\text{b)} \quad |F2(v,t,T)| \leq 3^m e^{-2vT}\{K(2T)^m e^{-2vT}(\frac{\alpha_1}{2vT} + \ldots + \frac{\alpha_{m+1}}{(2vT)^{m+1}})\} \tag{16}$$

if $m > o$ and $(m!)/2^m - 1 \leq 2vT$.

For the definition of c, m, K, α_1, ..., α_{m+1} see equations (7), (8) and (9). For the proof see [1] or [6].

Remarks: A comparison with the method of Durbin (see (8) and (9)) shows a reduction of the error bound by the factor $2e^{-2vT}$ for $m=o$ and $3^m e^{-2vT}$ for $m>o$. The condition $m!/2^m - 1 \leq 2vT$ might be difficult to fulfill for large m , and hence the application of the "Korrektur"-method is not recommended in such cases.

As mentioned before, an adequate reduction of the total error can be obtained by the "Korrektur"-method only if (for fixed N and T) the parameter v is suitable. This is illustrated in Fig. 1. It shows the error curves of the method of Durbin (F1 and FA) and of the "Korrektur"-method (F2 and FA). A success-

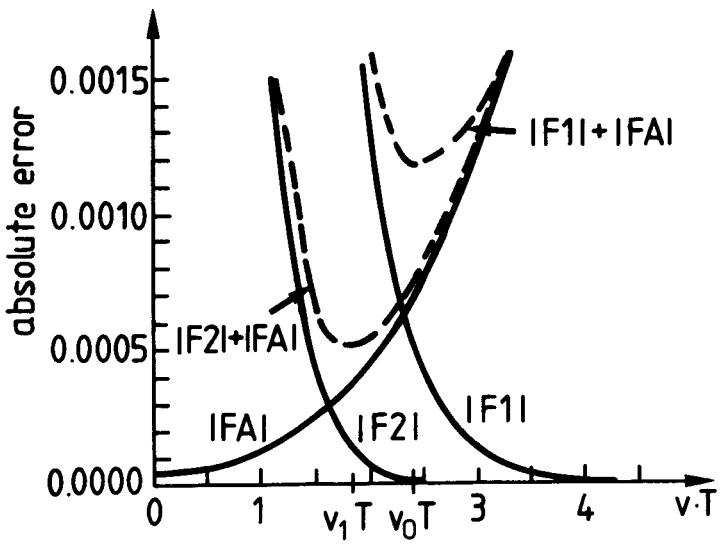

Fig. 1

ful application of the "Korrektur"-method requires a $v < v_o$. For $v > v_o$ the truncation error dominates and the reduced discretization error F2 does not lead to a noticeable reduction of the total error.

The opposite holds if the methods for the acceleration of convergence, that we describe in the following part, are applied. Acceleration of convergence is only sensible if $v \geq v_o$ or, which is the same, if the truncation error dominates.

However, a simultaneous application of an acceleration method and the "Korrektur"-method (as realized in the subroutine LAPIN) is recommended, if the parameters are optimally chosen by the procedures introduced in part 2.4.

2.3 Acceleration of convergence

In this part three acceleration methods used in the subroutine LAPIN (see chapter 3) are briefly described: The ε-algorithm, the minimum-maximum method and a method based on curve fitting. The latter is new, whereas the ε-algorithm was already used in [2] and [9], the minimum-maximum method in [1] in order to speed up the convergence of the series approximating the Laplace inversion integral. We have also tested other acceleration methods such as the Euler transformation, or Aitken's extrapolation procedure (see [8]). But these turned out to be less efficient than the above mentioned methods.
We can consider $f_N(t)$ (see (11)) for fixed t as a discrete function of N and define:

$f_N(t)$ as a function of N is monotonous if

$$|f_N(t) - f_\infty(t)| \geq |f_M(t) - f_\infty(t)|$$

for all N, M with $N \leq M$.

For a non-monotonous $f_N(t)$ the ε-algorithm (EPAL) and the minimum-maximum method (MINIMAX) in general significantly increase the rate of convergence. However, they fail - as do the Euler transformation and Aitken's extrapolation procedure - for a monotonous $f_N(t)$. The method based on curve fitting (CFM) leads in this case to a considerable improvement in the results.

With

$$c_k := \frac{e^{vt}}{T} \left[\mathrm{Re}\{F(v + \frac{ik\pi}{T})\} \cos \frac{k\pi t}{T} - \mathrm{Im}\{F(v + \frac{ik\pi}{T})\} \sin \frac{k\pi t}{T} \right] ,$$

$$k = 0,1,2,...$$

we can replace (11) by

$$f_N(t) = \frac{1}{2} c_o + \sum_{k=1}^{N} c_k . \qquad (17)$$

The *ε-algorithm* applied to (17) is defined as follows.

Let $N = 2q + 1$, $q \in \mathbb{N}$,

$$s_m := \sum_{k=1}^{m} c_k \quad \text{and}$$

$$\varepsilon_{p+1}^{(m)} := \varepsilon_{p-1}^{(m+1)} + 1/(\varepsilon_p^{(m+1)} - \varepsilon_p^{(m)})$$

$$\varepsilon_o^{(m)} := 0 \qquad (18)$$

$$\varepsilon_1^{(m)} := s_m ,$$

then the sequence $\varepsilon_1^{(1)}, \varepsilon_3^{(1)}, \varepsilon_5^{(1)}, \ldots, \varepsilon_{2q+1}^{(1)} = \varepsilon_N^{(1)}$, converges to $f_\infty(t) - c_o/2$. For a non-monotonous $f_N(t)$ in general it converges faster than the sequence of the partial sums s_m , $m = 1,2,...$ of the untransformed series.

The *minimum-maximum method* also increases the rate of convergence only in the case of a non-monotonous $f_N(t)$. The method works as follows. Having found three neighbouring stationary values of $f_N(t)$ as a function of N , say a maximum at $N = N1$ and $N = N3$, and a minimum at $N = N2$, an interpolating function for the maximum values at $N = N1$ and $N = N3$ is constructed. The mean value of the minimum at $N = N2$ and the

function value of the interpolating function at $N = N2$ yields the new approximation for $f_\infty(t)$. For a more detailed description of MINIMAX see [1].

The *method based on curve fitting* (CFM), applicable only for monotonous $f_N(t)$, consists in fitting the parameters of any function that has a horizontal asymptote $\gamma_A(x) \equiv \gamma$, by demanding that this function is an approximating function for the points $(N, f_N(t))$, $o \leq N_o \leq N \leq N_1$. The function value of the asymptote γ is the desired approximation for $f(t)$. With the simple rational function

$$r(x) := \frac{\alpha}{x^2} + \frac{\beta}{x} + \gamma \ , \qquad (19)$$

for example, we achieved high accuracy already for small N_1. The CFM fills an important gap: now it is also possible to speed up the convergence of the Fourier series (5) in case of a monotonous $f_N(t)$ [4]. The subroutine LAPIN (see part 3.2) automatically chooses between CFM and EPAL (MINIMAX) depending on whether $f_N(t)$ is a monotonous or a non-monotonous function of N. Tests have shown that for non-monotonous $f_N(t)$ EPAL mostly is superior to MINIMAX in accuracy. However, we found examples where the ε-algorithm falsifies the results, but the minimum-maximum method did not. In these cases, the subroutine LAPIN chooses by itself the MINIMAX method to accelerate the convergence of the series (for more details, see part 3.2, significance of the parameter H). Furthermore, the ε-algorithm is not applicable for arbitrarily large N in (17), because of overflows occurring in (18) for larger N.

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[4] For instance, $f_N(t_o)$ often is a monotonous function of N, if $f(t)$ is a step function with the discontinuity at t_o.

2.4 The choice of optimal parameters

We already mentioned that a good choice of the free parameters N and CON = vT is not only important for the accuracy of the results but also for the application of the "Korrektur"-method and the methods for the acceleration of convergence (see Fig. 1). These methods do not improve the result if the parameters are chosen badly.

Two methods are now presented which approximately determine the 'optimal' v for fixed N and T . The main difference between the two methods is the definition of 'optimal parameters'.

Definition A: For fixed N and T the parameter v of the method of Durbin (see (12)), with or without the application of the "Korrektur"-method or a method for the acceleration of convergence, is optimal if the absolute values of discretization and truncation error are equal.

Definition B: For fixed N and T the parameter v of the above mentioned methods (see definition A) is optimal if the sum of the absolute values of discretization and truncation error is minimal (see Fig. 1, where the optimal v is given by v_o and v_1).

Method A: Let $\bar{f}_N(t)$, $\bar{f}_{NK}(t)$ be the approximate values for f(t) computed by the method of Durbin (12) and the "Korrektur"-method (13), respectively. The bar indicates that one of the methods for the acceleration of convergence may have been applied.

Let $R(N,v,t,T)$ be the expression in the brackets on the right side of (1o). Neglecting the dependence of v in R we can write for fixed t,T : $R(N,v,t,T) \cong R(N)\cdot\delta$, where $\delta \varepsilon [-1,+1]$ indicates the application of an acceleration method ($\delta \equiv 1$ if none of the acceleration methods is used). The truncation error of $\bar{f}_N(t)$ or $\bar{f}_{NK}(t)$ is therefore given by

$$FA(N,v,t,T) \cong \frac{e^{vt}}{T} R(N)\delta \ . \tag{2o}$$

With (5), (6) and (2o) we find

$$\bar{f}_N(t) \cong f(t) - \frac{e^{vt}}{T} R(N)\delta + O(e^{-2vT}) \ . \tag{21}$$

Let v_1, v_2 be large and $v_1 \neq v_2$ [5], then

$$\bar{f}^1_N(t) - \bar{f}^2_N(t) \cong R(N)\delta\cdot(e^{v_2 t} - e^{v_1 t})/T \tag{22}$$

or

$$R(N)\delta \cong T \frac{\bar{f}^1_N(t) - \bar{f}^2_N(t)}{e^{v_2 t} - e^{v_1 t}} \ . \tag{23a}$$

Similarly we get for the "Korrektur"-method

$$R(N)\delta \cong T \frac{\bar{f}^1_{NK}(t) - \bar{f}^2_{NK}(t)}{e^{v_2 t} - e^{v_1 t}} \ . \tag{23b}$$

The discretization error (6) of the method of Durbin can be written as [3]

$$F1(v,t,T) = e^{-2vT} f(2T + t) + O(e^{-4vT}) \ . \tag{24a}$$

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[5] We found that for example $v_1 := 2o$, $v_2 := v_1 - 2$ is a good choice.

From (13) we find for the discretization error of the "Korrektur"-method

$$F2(v,t,T) = \sum_{k=2}^{\infty} e^{-2vTk}\{f(2kT+t) - f(2T(3k-2)+t)\} .$$

Hence [3]

$$F2(v,t,T) = e^{-4vT}\{f(4T+t) - f(8T+t)\} + O(e^{-6vT}) . \quad (24b)$$

Using definition A, the equations (23) and (24) easily lead to the following equations for the optimal parameter $v = v_{OPT}^{A}$:

$$v_{OPT}^{A} \cong - \frac{1}{2T + t} \ln \left| \frac{R(N)\delta}{T\, \bar{f}_N(2T+t)} \right| , \quad (25a)$$

(method of Durbin)

and

$$v_{OPT}^{A} \cong - \frac{1}{4T+t} \ln \left| \frac{R(N)\delta}{T\{\bar{f}_N(4T+t) - \bar{f}_N(8T+t)\}} \right| . \quad (25b)$$

("Korrektur"-method)

Because of definition A the total absolute error $|f(t)-\bar{f}_N(t)|$ or $|f(t)-\bar{f}_{NK}(t)|$ for $v=v_{OPT}^{A}$ is approximately given by

$$TERR \cong 2 \frac{e^{v_{OPT}^{A} \cdot t}}{T} |R(N)\delta| . \quad (26)$$

Method B: We now use definition B and assume that $R(N,v,t,T)$ is no longer a constant function of v to get a more accurate approximation formula for v_{OPT} .

The dependence of v is assumed to be as follows ($R(N,v,t,T) = R(N,v)\delta$ because t,T are fixed, $v_1>o$ arbitrary):

$$R(N,v)\delta \cong R(N,v_1)\delta \cdot \Big[\mathrm{Re}\{F(v + i\tfrac{N\pi}{T})\} \cos \tfrac{N\pi t}{T} - \mathrm{Im}\{F(v + i\tfrac{N\pi}{T})\} \sin \tfrac{N\pi t}{T}\Big] \Big/ \Big[\mathrm{Re}\{F(v_1 + i\tfrac{N\pi}{T})\} \cos \tfrac{N\pi t}{T} - \mathrm{Im}\{F(v_1 + i\tfrac{N\pi}{T})\} \sin \tfrac{N\pi t}{T}\Big] \; . \tag{27}$$

The acceleration factor δ can be computed very easily from (23a) without additional function evaluations:

$$\delta = \frac{\bar{f}_N^1(t) - \bar{f}_N^2(t)}{f_N^1(t) - f_N^2(t)} \; . \tag{28}$$

Let $AR(v_1,v,N)$ be the expression in brackets on the right side of (27) and $R(N,v_1)\delta := R(N)\delta$, where $R(N)\delta$ is computed by method A. Then (27) is expressible in the form

$$R(N,v)\delta = R(N)\delta \cdot AR(v_1,v,N) \; . \tag{29}$$

Definition B implies (for the method of Durbin):

$$\frac{\partial}{\partial v}\left[\, |R(N,v)\delta| \frac{e^{vt}}{T} + |F1(v,t,T)| \,\right]_{|v=v_{OPT}^B} = o \; . \tag{3o}$$

Approximating the derivative of $R(N,v)$ by finite differences, we find the following iteration procedure to solve equation (3o):

$$\left[\frac{\partial}{\partial v} R(N,v)\right]^{(i)} \cong \frac{R(N,v^{(i-1)}) - R(N,v_1^{(i-1)})}{v^{(i-1)} - v_1^{(i-1)}} \; , \quad i = 1,2,\ldots,s \; , \tag{31a}$$

$$v^{(o)} = v_{OPT}^A \; , \quad v_1^{(o)} = v_1 \tag{31b}$$

$$v_1^{(i)} = v^{(i-1)} \; , \quad i = 1,\ldots,s-1 \; . \tag{31c}$$

$$v^{(i)} = -\frac{1}{2T + t} \ln \left[\frac{\frac{\partial}{\partial v} |R(N,v)^{(i)}| \ \delta + |R(N,v^{(i-1)})| \delta \cdot t}{2T^2 |\bar{f}_N(2T + t)|} \right],$$

$$i = 1,2,\ldots,s \ . \qquad (31d)$$

In (31b) v_{OPT}^A and v_1 are defined by method A (see equation (25) and (22), respectively). Equation (31d) follows from (3o) substituting (31a) for the derivative of $R(N,v)$ and (24a) for $F1(v,t,T)$.

Hence the optimal parameter $v = v_{OPT}^B$ for fixed N,T,t is given by

$$v_{OPT}^B := v^{(s)} \ . \qquad (32)$$

An analogous result holds for the "Korrektur"-method: Replacing F1 by F2 in (3o), we only have to substitute (31d) by

$$v^{(i)} = -\frac{1}{4T + t} \ln \left[\frac{\left[\frac{\partial}{\partial v} |R(N,v)^{(i)}| \ \delta + |R(N,v^{(i-1)})| \delta \cdot t \right.}{4T^2 |\bar{f}_N(4T+t) - \bar{f}_N(8T+t)|} \right],$$

$$i = 1,2,\ldots,s \ . \qquad (31e)$$

It is sufficient to choose $s=1$ or $s=2$, as numerical tests have shown.

Again it is possible to compute approximately an upper bound for the total error, if the parameter $v = v_{OPT}^B$ is used for the computation of $\bar{f}_N(t)$ [6].

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6) A similar equation holds for $\bar{f}_{NK}(t)$.

We find

$$TERR \cong \frac{e^{v_{OPT}^{B} \cdot t}}{T} \left| R(N, v_{OPT}^{B}) \right| \delta + e^{-2v_{OPT}^{B} \cdot T} \left| \bar{f}_N(2T+t) \right| . \quad (33)$$

Remarks: The simplifications made in order to derive the equations (25) and (31) do in general not cause any difficulties. Besides a few exceptions, which are discussed later, the optimal parameters v_{OPT}^{A} and v_{OPT}^{B} are a good approximation for the true optimal parameters.

If the ε-algorithm is used in order to accelerate the convergence of the series (5), it is not possible to compute the acceleration factor δ for large N with the desired accuracy (the ε-algorithm breaks down after a certain $N_o < N$ depending on v,t and T ; N_o is not known in advance; see also the final remarks of part 2.3). Therefore the minimum-maximum method allows a more accurate determination of the optimal parameters by method A or B, and hence of the total error (26) or (33).

3. The subroutine LAPIN

In this chapter the subroutine LAPIN - introduced in [7] - is described.
We further give several examples to demonstrate how LAPIN can be applied successfully. Especially problems arising if one of the acceleration methods is used are discussed.
The examples show that a correct application of LAPIN leads to a high accuracy in the results and that misleading results can be avoided by simple manipulations of the parameters.

3.1 Description of the subroutine LAPIN

(a) Purpose

Suppose f(t) is a real function and F(s) its Laplace transform, that has no singularities to the right of the origin, then the subroutine LAPIN calculates from F(s) for a programmers-chosen set of t-values, the corresponding values for f(t) , using the above described algorithms.

(b) Usage

```
CALL LAPIN(F,T1,TN,N,IMAN,ILAPIN,IKONV,NS1,NS2,ICON,IKOR,
                                              CON,H,E,IER)
```

(c) Description of the parameters

Type:

INTEGER*4 N,IMAN,ILAPIN,IKONV,NS1,NS2,ICON,IKOR,IER

REAL*8 T1,TN,CON,H,E

COMPLEX*16 F

Input parameters: T1,TN,N,IMAN,ILAPIN,IKONV,NS1,NS2,ICON,IKOR,CON

Output parameters: H,IER

Significance of the parameters

F — Laplace transform - external function, to declare as EXTERNAL in the calling program ;

T1,TN — lower and upper bound of the interval in which f(t) shall be approximated;

N — number of t-values for which f(t) shall be computed, the t-values are given by

t_k = T1 + (TN-T1)k/(N+1) , k = 1(1)N;

IMAN — = o , all further parameters are placed automatically, except NS1, which has to be set equal to 6o;

= 1 , a manual choice of the following parameters is possible;

ILAPIN — If ILAPIN = 1 , the approximate value $f_N(t)$ (see 11) is computed with T=t,

if ILAPIN = 2 with T=TN (T=2TN for the "Korrektur"-terms). For T=t the computation of sine and cosine terms and of the imaginary parts of F(s) in (11) is cancelled, on the other hand Re{F(s)} becomes dependent on t . Hence ILAPIN = 1 is recommended if the inverse is computed only for a few t-values.

IKONV — IKONV = 1 implies the use of the acceleration method MINIMAX, IKONV = 2 the acceleration of convergence with EPAL. In both cases the subroutine automatically chooses the curve fitting method (CFM) for monotonous $f_N(t)$.

NS1 number of function evaluations of F(s) used to approximate f(t) ($f_N(t) = f_{NS1}(t)$) ;

NS2 number of function evaluations of F(s) used to approximate the "Korrektur"-term f(2T+t) ($f_N(2T+t) = f_{NS2}(2T+t)$) ;

ICON = o no optimal choice of the free parameters,

= 1 optimal choice of the free parameters for $t = t_{[N/2]}$

= 2 optimal choice of the free parameters for $t = t_k$, $k = 1(1)N$;

an optimal choice of the free parameters is found by using method A or B (see part 2.4) to compute an optimal v for a given NS1.

If ICON = 1 the optimal v at $t = t_{[N/2]}$ is used for the computation of all $f(t_k)$, $k = 1(1)N$.

IKOR = o no application of the "Korrektur"-method,

= 1 application of the "Korrektur"-method;

CON by the choice of CON = vT , the free parameter v is determined in case that ICON = o ;

H matrix of dimension 6 by N , contains on return in the

1st row the approximation values for $f(t_k)$, k = 1(1)N ;

2nd row work area;

3rd row the computed optimal parameter $CON_{OPT} = v_{OPT} \cdot T$ for $t = t_k$, k = 1(1)N , ($CON_{OPT} = 18$ if the truncation error (23) is zero, $CON_{OPT} = 1$ if the discretization error (24) is zero or of very small absolute value);

4th row the code for the used acceleration method:

= o no acceleration of convergence,

= 1 MINIMAX,

= 2 EPAL,

= 3 CFM,

= P $\geq$ 4 EPAL, overflow occurred after P-2 iterations (NS1= P-2 values of F(s) are used for the approximation of f(t)); note: the output parameter on the 4th row of H may be different from the input parameter IKONV . The subroutine LAPIN always uses

(a) CFM if $f_N(t)$ is monotonous in N ,

(b) MINIMAX if the application of EPAL falsifies the results,

(c) no acceleration method if only 1 or 2 stationary values of $f_N(t)$ as a function of N are found;

5th row absolute error calculated by (33) if ICON = 2 and ILAPIN = 1; if ICON = 1 the error estimation is valid only at $t = t_{[N/2]}$;

6th row contains a control number of up to 6 digits ($n_1 n_2 n_3 n_4 n_5 n_6$), the digits refer to the used auxiliary quantities, the "Korrektur"-term $f_{NS2}(2t_1+t_o)$ and to

$f_{NS1}(t)$ as follows (see Table 2 for the definition of t_o and t_1):

$n_1 \rightarrow f^1_{NS1}(t_o)$ (CON = 2o)

$n_2 \rightarrow f^2_{NS1}(t_o)$ (CON = 18)

$n_3 \rightarrow f_{NS1}(2t_1+t_o)$

$n_4 \rightarrow f_{NS1}(4t_1+t_o)$

$n_5 \rightarrow f_{NS1}(8t_1+t_o)$

$n_6 = n_{61}+n_{62}$; $n_{61} \rightarrow f_{NS1}(t_o)$; $n_{62} \rightarrow f_{NS2}(2t_1+t_o)$.

If one of the digits is zero the application of the ε-algorithm falsifies the results of the corresponding auxiliary quantity (MINIMAX is used). Otherwise the digits are equal to 1 (besides n_{62}, which is equal to 2).

Note: $n_3 = o$ always if IKOR = 1, $n_4 = n_5 = o$ always if IKOR = o.

Whenever a zero in the control number indicates the falsification of the results, it is recommended to increase NS1 or NS2.

E matrix of dimension 3 by NS1, work area;

IER error parameter, control of input data:

= o no error ,

= 1 TN < T1

= 1o N < 1 ,

= 1oo IMAN < o or IMAN > 1 ,

= 1ooo ILAPIN < 1 or ILAPIN > 2 ,

= 1oooo IKONV < 1 or IKONV > 2 ,

= 1ooooo NS1 < 1 or (NS2 < 1 and IKOR = 1) ,

= 1oooooo ICON < o or ICON > 2 or (ICON = 2 and ILAPIN = 2) ,

= 1ooooooo IKOR < o or IKOR > 1 ,

= 1oooooooo CON $\leq$ o .

E.g. IER = 11 means that 1 and 1o occurred.

3.2 The application of LAPIN

3.2.1 General remarks

The following table shows the possible combinations of the above described algorithms offered by the subroutine LAPIN.

	ILAPIN	ICON	IKOR	IKONV
IMAN = 1	1	o/1/2	o/1	1/2
	2	o/1	o/1	1/2
IMAN = o	1	1	o	2

Table 1

The method A for an optimal choice of the free parameters is used if ILAPIN = 2 , method B if ILAPIN = 1 .

The application of the "Korrektur"-method is not recommended first, in the case that the absolute value of the "Korrektur"-term $f(2T + t)$ is small or equal to zero: $|f(2T + t)| << 1$, (no noticeable improvement of the accuracy occurs), and second, if $f(t)$ is a rapidly increasing function as $t \to \infty$ (see the remarks to theorem 2.1).

The same holds for the application of the methods for an

optimal choice of the free parameters if the auxiliary quantities (these are f(2T+t) in (24a) and f(4T+t) , f(8T+t) , in (24b)) are equal to zero. Although the denominators in (25) do not vanish (because of the discretization and truncation errors), the computed optimal parameters might be misleading. In these cases, it is very helpful to have a global conception about the Laplace inverse f(t) . If not already known, this can be obtained easily by the subroutine LAPIN choosing either IMAN = o or IMAN = 1 , ILAPIN = 2 , ICON = o , IKOR = o and IKONV = 1 . The latter combination of the parameters coincides with the method of Durbin in connection with the MINIMAX-method in order to speed up the convergence of the Fourier series.

Let NS1 be the number of function evaluations of F(s) used to approximate f(t) and NS2 the number of function evaluations used to approximate the "Korrektur"-term f(2T+t) . For given NS1 we found that $NS1/2 \leq NS2 \leq NS1$ if $NS1 \leq 1oo$ and $NS1/1o \leq NS2 \leq NS1/2$ if $NS1 \geq 1oo$ is a good choice for NS2. As stated above, the occurrence of overflows in (18) often makes it impossible to transform a given number NS1 of terms of the series (17) by the ε-algorithm. If it breaks down after $N < NS1$ iterations the accuracy for the determination of the optimal parameters and the total error (33) is diminished. The MINIMAX-algorithm does not cause such problems.

Finally, we would like to mention that it can be necessary to know in advance the s-values for which F(s) has to be evaluated (for instance, if F(s) is a solution of a differential or integral equation which is not given analytically). These s-values are defined by T and CON = v·T ($s = v+ik\pi/T$, k = o(1)NSUM).

In Table 2, the values of CON and T are listed, for which the 'auxiliary quantities' ($f_{NS1}(T)$) must be computed.

T	t_o	t_o	$2t_1+t_o$	$4t_1+t_o$	$8t_1+t_o$
CON	20	18	5	5	5

	ILAPIN = 1 ICON = 1	ILAPIN = 2 ICON = 1	ILAPIN = 1 ICON = 2
t_o	$T1+(TN-T1)\left[\frac{N}{2}\right]/(N+1)$	$T1+(TN-T1)\left[\frac{N}{2}\right]/(N+1)$	$T1+k(TN-T1)/(N+1)$, $k=1(1)N$ [7]
t_1	$T1+(TN-T1)\left[\frac{N}{2}\right]/(N+1)$	TN	$T1+k(TN-T1)/(N+1)$, $k=1(1)N$ [7]

Table 2

If ICON = o no auxiliary quantities are needed. If ICON > o, IKOR = o requires the computation of $f_{NS1}(t_o)$ and $f_{NS1}(2t_1+t_o)$, IKOR = 1 the computation of $f_{NS1}(t_o)$, $f_{NS1}(4t_1+t_o)$ and $f_{NS1}(8t_1+t_o)$ with the above given values of CON, t_o and t_1.

3.2.2 On the influence of the parameter CON on the discretization and truncation error

The influence of the choice of CON = vT on the accuracy of the results was already mentioned. We now consider the approximate value $f_N(t)$ (see (11) or (14)) as a function of N (t fixed).

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[7] N = number of t-values for which f(t) shall be approximated.

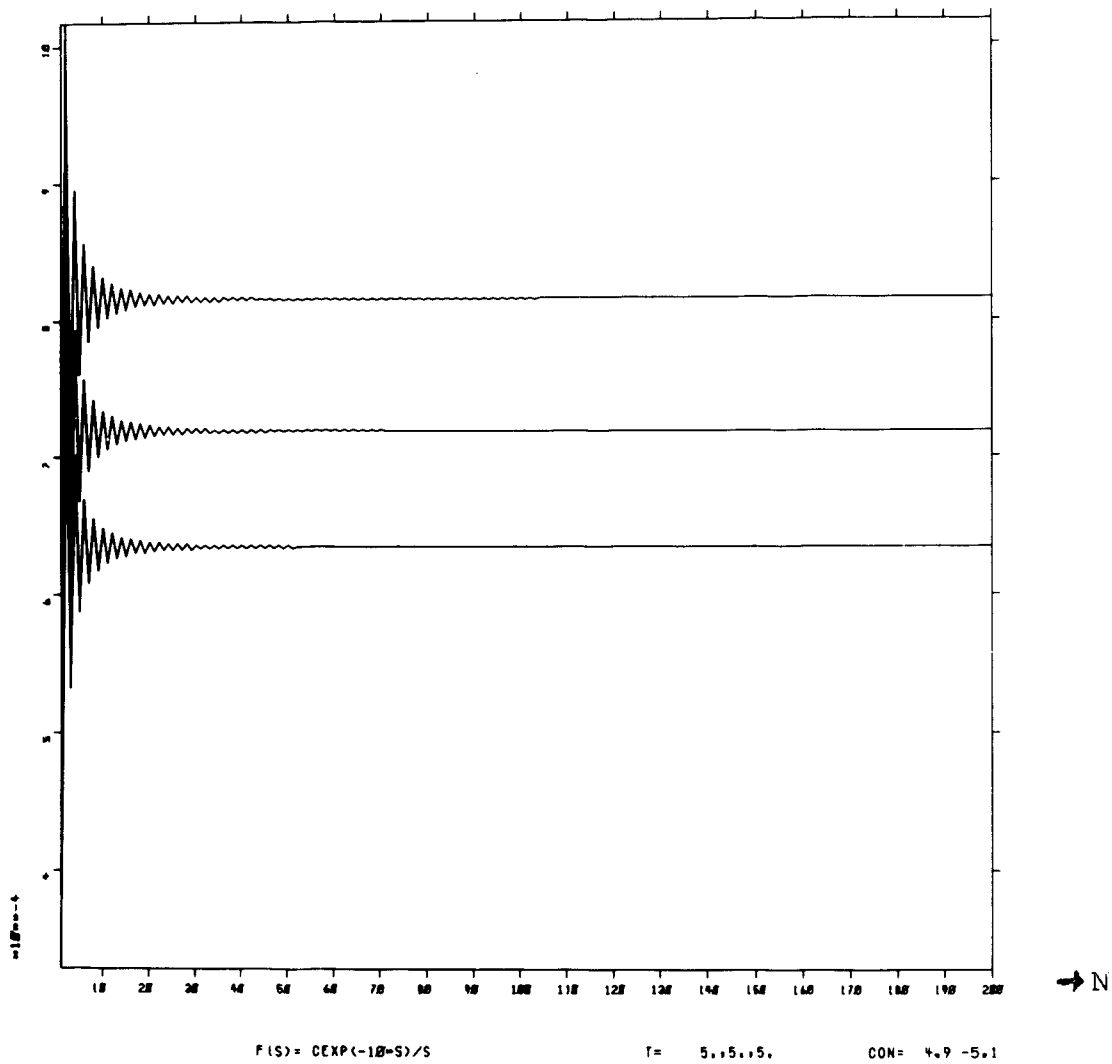

Fig. 2

Fig. 2 shows $f_N(t)$, N=o(1)2oo approximating the Laplace inverse of F(s)=exp(-1os)/s at t=5 with three different values of CON: CON=4.9; 5.o; 5.1. The effect is obvious. The discretization error $|f_\infty(5)-f(5)|=|f_\infty(5)|$ is smallest for CON=5.1 (note: f(5)=o and $f_\infty(5)\cong f_{2oo}(5)$ in Fig. 2).

3.2.3 The application of the acceleration methods

The three methods for the acceleration of convergence of the Fourier series described in part 2.3 are available in the subroutine LAPIN. The parameter IKONV (see part 3.1) decides which of the methods is used.
It is in general impossible to know in advance which of these methods is most efficient for a given problem.
However we can give some hints that allow the application of the most suitable method for a big class of Laplace transforms:

1. If $f_N(t)$ is a monotonous function of N, the only algorithm reducing the truncation error is CFM. Therefore LAPIN automatically chooses CFM in this case independent of the choice of the parameter IKONV. By IKONV it is only possible to select between MINIMAX and EPAL.
2. Using the same number of function evaluations EPAL is mostly superior to MINIMAX in accuracy. If the desired accuracy needs not to be very high the use of MINIMAX is advantageous: It is faster than EPAL and the determination of the optimal parameters is more accurate.
   EPAL is especially recommended if the evaluation of $F(s)$ is time consuming.

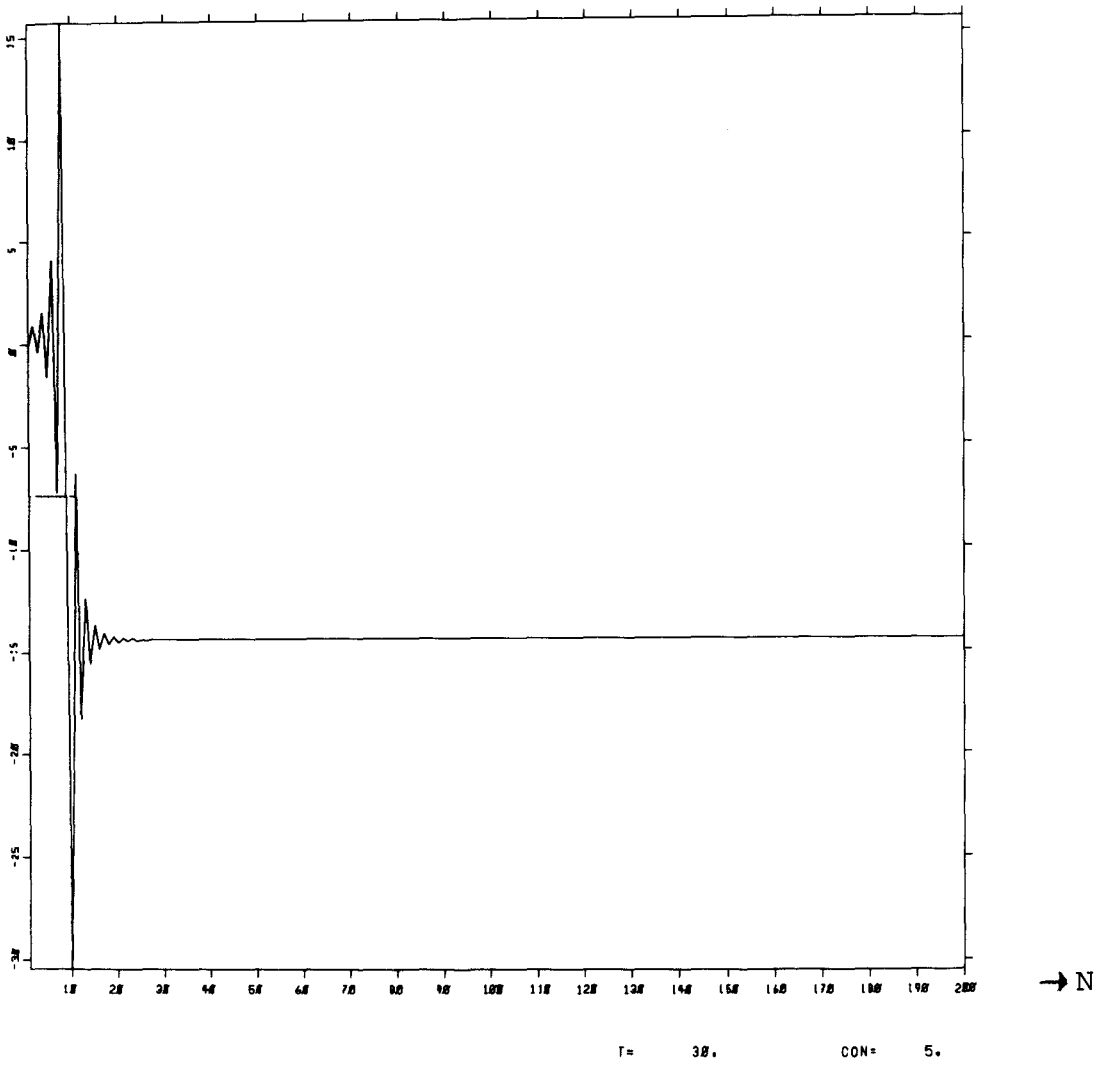

Fig. 3

3. EPAL may falsify the results. To detect at least a big class of these cases, the 'control number' H(6,•) was introduced (see part 3.1.3-6th row of the parameter H). The digit referring to a t-value where $f_N(t)$ might be falsified by the application of the ε-algorithm is equal to zero. (In fact the control digit is zero always for $N_o<N<3N_o$ - see also p. 31 and footnote on p. 35).

Figs. 3 and 4 show $f_N(t)$ as a function of N with

$F(s) = s\cdot(s^2 + 1)^{-2}$.

With t=3o and CON=5 $f_N(t)$ has a 'step' at N_o=1o

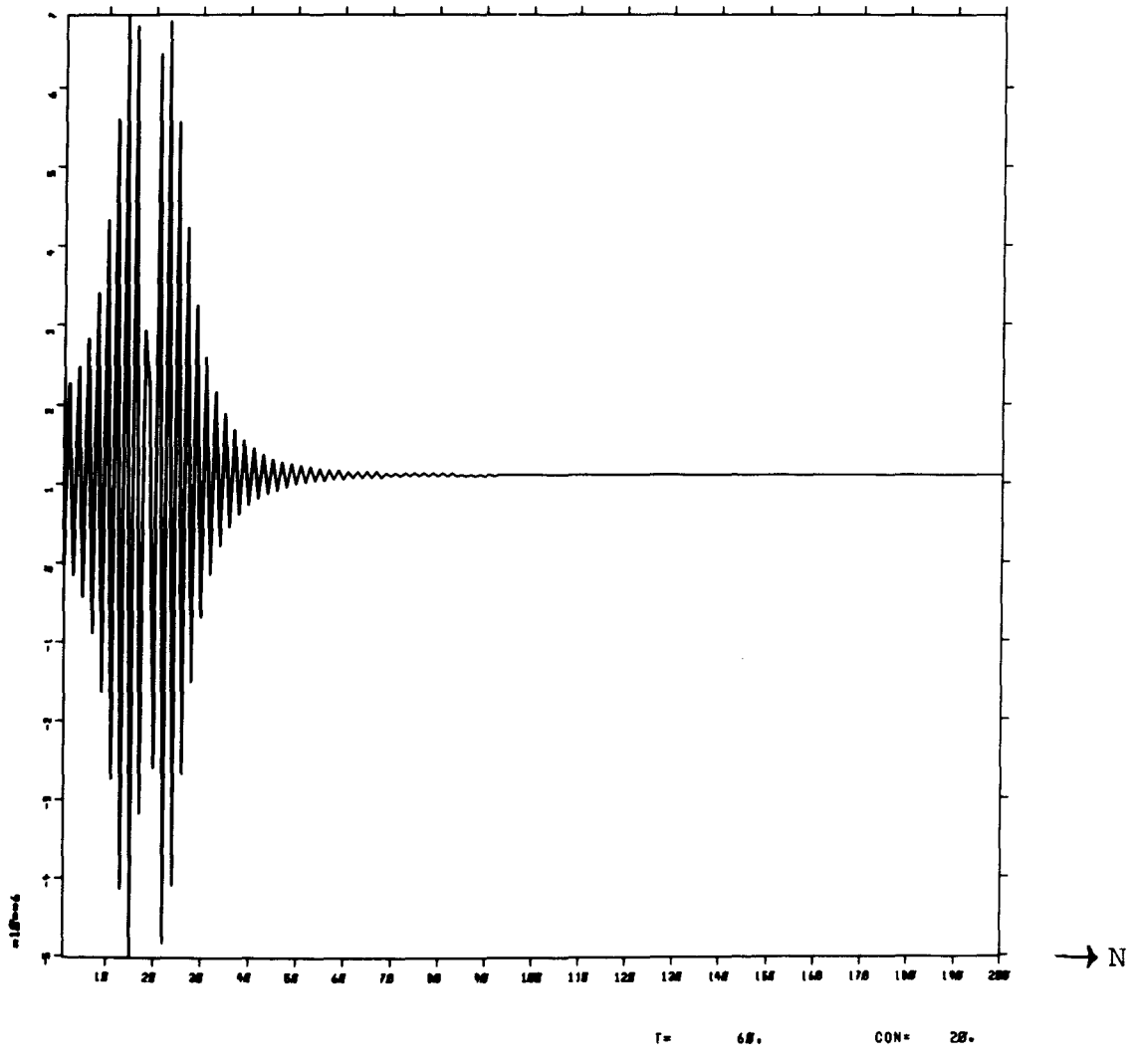

Fig. 4

(see Fig. 3). If such a step occurs, a falsification of the result is possible for $N<3N_o$ [8]. Hence, in our example in Fig. 3 the control digit is equal to zero for $N<3o$. The same holds for the example demonstrated in Fig. 4. For $N\leq 2o$ the stationary values of $f_N(6o)$ are increasing.

The control digit is zero unless $N>6o$. If a control digit is zero LAPIN automatically uses the MINIMAX method.

In part 3.3 we show by an example how to use the control number to avoid misleading results.

---

[8] This result was obtained be numerical tests. We never detected a falsification at the results for $N>3N_o$.

The control digit is zero always if $N_o<N<3N_o$, and one otherwise.

3.3 Numerical examples [9]

From the following examples one can get some idea of the accuracy of the subroutine LAPIN and the possibilities it offers to find an 'optimal' solution for a given problem by a suitable choice of the different algorithms described above. The parameters used in the following tables are defined in part 3.1. The code numbers refer to the parameters ILAPIN-ICON-IKOR-IKONV (1-2-o-1, for example, means: ILAPIN=1, ICON=2, IKOR=o and IKONV=1). IMAN=o coincides with 1-1-o-2.

Table 3 shows the errors occurring if $F(s) = s(s^2+1)^{-2}$ is inverted. Three different parameter combinations of LAPIN are

$F(t) = t \cdot \sin(t)/2$, $F(s) = s(s^2+1)^{-2}$

method	Durbin (v·T=5)	L A P I N			
Code		2-1-o-1	IMAN=o	1-2-1-1	
NS1+NS2	2ooo	3o	6o	16o+4o	
		real absolute error			absolute error by (33)
t 1	0.4 D-02	0.2 D-02	0.1 D-11	0.351 D-10	0.273 D-10
3	0.6 D-01	0.1 D-01	0.1 D-11	0.211 D-09	0.236 D-09
5	0.1 D-01	0.2 D-02	0.1 D-12	0.573 D-09	0.648 D-09
7	0.8 D-01	0.9 D-02	0.2 D-09	0.786 D-09	0.979 D-09
9	0.2 D-01	0.9 D-03	0.1 D-10	0.774 D-09	0.191 D-08
11	0.1 D-01	0.3 D-03	0.2 D-10	0.590 D-09	0.273 D-08
13	0.6 D-01	0.2 D-01	0.9 D-10	0.107 D-08	0.372 D-08
15	0.5 D-02	0.1 D-01	0.2 D-09	0.175 D-08	0.356 D-08
17	0.7 D-02	0.2 D-01	0.1 D-09	0.225 D-08	0.569 D-08
19	0.1 D-00	0.5 D-02	0.4 D-10	0.321 D-09	0.633 D-08
CPU-time sec (for t=1(1)20)	1.21	0.04	0.42	1.14	

Table 3

[9] All calculations were performed in double precision on the IBM 370/168 computer of KFA Jülich.

compared with the method of Durbin. With only a few function evaluations of F(s) and little CPU-time, LAPIN computes the Laplace inverse with a considerable accuracy. For instance, the first two columns show that the method of Durbin needs about 60 times more function evaluations and 30 times more CPU-time than LAPIN to get a comparable accuracy. Column 3 shows - and this was confirmed by many other examples - that using the subroutine LAPIN as a 'black box' (IMAN=0) yields excellent results. From a comparison between columns 4 and 5 it is obvious that the absolute error computed by (33) is a good approximation for the real error (such an error estimation is only possible if ICON=2; it is most accurate for IKONV=1).
As a second example, the Laplace transform of the step function

$$U(t-10) := \begin{cases} 0 & t < 10 \\ 0.5 & t = 10 \\ 1 & t > 10 \end{cases}$$

was inverted (see Table 4). Comparing the results of Durbin with

$f(t) = U(t-10)$, $F(s) = \exp(-10s)/s$

method	Durbin (v·T=5)	L A P I N			LAPIN
Code		2-1-0-1	IMAN=0		1-2-1-2
NS1+NS2	2000	50	60		350+150
	real absolute error				real absolute error
t 5	0.6 D-02	0.4 D-05	0.5 D-06	t 9.0	0.1 D-13
6	0.6 D-02	0.1 D-04	0.5 D-06	9.2	0.3 D-12
7	0.6 D-02	0.6 D-04	0.5 D-06	9.4	0.8 D-14
8	0.7 D-02	0.5 D-03	0.5 D-06	9.6	0.1 D-09
9	0.7 D-02	0.1 D-01	0.6 D-06	9.8	0.6 D-05
10	0.6 D-02	0.5 D-04*	0.6 D-06*	10.0	0.3 D-09*
11	0.5 D-02	0.3 D-01	0.8 D-05	10.2	0.1 D-05
12	0.6 D-02	0.6 D-02	0.5 D-06	10.4	0.8 D-10
13	0.6 D-02	0.1 D-02	0.5 D-06	10.6	0.2 D-09
14	0.6 D-02	0.1 D-02	0.5 D-06	10.8	0.8 D-10
15	0.6 D-02	0.2 D-02	0.5 D-06	11.0	0.2 D-12
CPU-time sec (for t=1(1)20)	2.02	0.06	0.32	CPU-time sec	13.70

* CFM was used to accelerate convergence.

Table 4

those obtained from LAPIN we come to the same conclusion as in the example above. The high accuracy at $t = 1o$ is possible only if the curve-fitting method is used to speed up the convergence of the series. EPAL and MINIMAX fail because $f_N(1o)$ is monotonous in N. But also at points very close to the discontinuity at $t = 1o$ a high accuracy is obtained by LAPIN as demonstrated in the last column of Table 4.

$f(t) = (-t^3+9t^2-18t+6)/6$, $F(s) = (s-1)^3/s^4$

method	LAPIN			LAPIN		
code	1-2-o-2 (without Korrektur)			1-2-1-2 (with Korrektur)		
NS1+NS2	1oo			6o+4o		
	absolute error real	absolute error by (33)	$v_{OPT}\cdot T$	absolute error real	absolute error by (33)	$v_{OPT}\cdot T$
t 1	0.1 D-10	0.2 D-10	12.2	0.3 D-12	0.4 D-14	9.4
3	0.9 D-10	0.1 D-10	14.7	0.6 D-12	0.5 D-13	9.9
6	0.1 D-09	0.2 D-10	15.4	0.2 D-12	0.2 D-12	10.1
9	0.5 D-10	0.7 D-10	16.0	0.8 D-13	0.1 D-12	10.5
CPU-time sec (t=1(1)1o)	1.49			0.81		

Table 5

From Table 5 one gets some idea of the effect of the"Korrektur"-method. It can be seen that (with the same number of function evaluations) the"Korrektur"-method (right part of Table 5) is clearly more accurate. This is not only caused by the reduction of the discretization error. The optimal parameter $v_{OPT}\cdot T$ is smaller if the"Korrektur"-method is applied. Hence the truncation error is reduced too.

As a further example, we show in Table 6 the dependence of the optimal parameter v_{OPT} on the number NS1 of function evaluations (v_{OPT} also depends on t). It is obvious that primarily

$f(t) = 1-\exp(t)\operatorname{erfc}(\sqrt{t})$; $F(s) = 1/(s(\sqrt{s}+1))$

method code	LAPIN 1-2-o-2		
NS1	absolute error at t=1 real	by (33)	$v_{OPT}\cdot T$
1o	0.103 D-04	0.416 D-05	6.61
2o	0.352 D-10	0.900 D-10	11.96
3o	0.356 D-11	0.801 D-11	13.16

Table 6

the possibility to calculate v_{OPT} for a given NS1 (and NS2) makes the inversion methods based on Fourier series expansions accurate and efficient.

We now want to explain how to avoid a falsification of the results by the application of an acceleration method[1o].

As already mentioned, the necessary informations can be taken from the control number H(6,•) (see parts 3.1.3 and 3.2.3). The Laplace transform $F(s) = L[t\cdot\sin(t)/2] = s(s^2 + 1)^{-2}$ is inverted using different parameters in the subroutine LAPIN. The results for 7 different values of NS1 and NS2 are

---

[1o] Falsification of the result means, that the approximation by the accelerated series is worse than that of the original series. The application of the MINIMAX-algorithm (differently from EPAL) does not involve such a falsification.
On the other hand misleading results are always obtained if $N<N_o$, regardless whether an acceleration method is applied or not (step at $N=N_o$).

method code			LAPIN 1 - 2 - 1 - 1			
Line number	NS1	NS2	absolute error for t=2o real	by (33)	CON_{OPT}	control number [11]
1	4o	1o	o.179D-o2	o.459D-o5	4.3	1 1 o o 1 3
2	8o	2o	o.268D-o3	o.181D-o6	5.2	1 1 o o o 3
3	8o	4o	o.1o5D-o6	o.181D-o6	5.2	1 1 o o o 1
4	8o	6o	o.873D-o7	o.181D-o6	5.2	1 1 o o o 3
5	16o	4o	o.539D-o8	o.672D-o8	6.o	1 1 o 1 o 1
6	16o	8o	o.378D-o8	o.672D-o8	6.o	1 1 o 1 o 3
7	2oo	1oo	o.132D-o8	o.234D-o8	6.3	1 1 o 1 1 3

control digit for $f_N(2o)$; CON=2o (see Fig. 5)

" $f_N(2o)$; CON=18;

" $f_N(6o)$; (without significance because IKOR=1)

" $f_N(1oo)$; CON=5 (see Fig. 6)

" $f_N(18o)$; CON=5 (see Fig. 7)

" $f_N(2o)$; $f_N(6o)$; $CON=CON_{OPT}$ (see Fig. 8/9)

Table 7

listed in Table 7. The control digits for the auxiliary quantities $f_N(2o)$ with CON=2o and $f_N(2o)$ with CON=18 (necessary for the computation of the truncation error)

[11] It should be mentioned that it is impossible to detect a 'step' at $N=N_o$ if $N<N_o$. Therefore the 5th digit of the control number in line 1 - for example - is equal to one (no 'step' for $f_N(18o)$ if $N<55$, see Fig. 7).

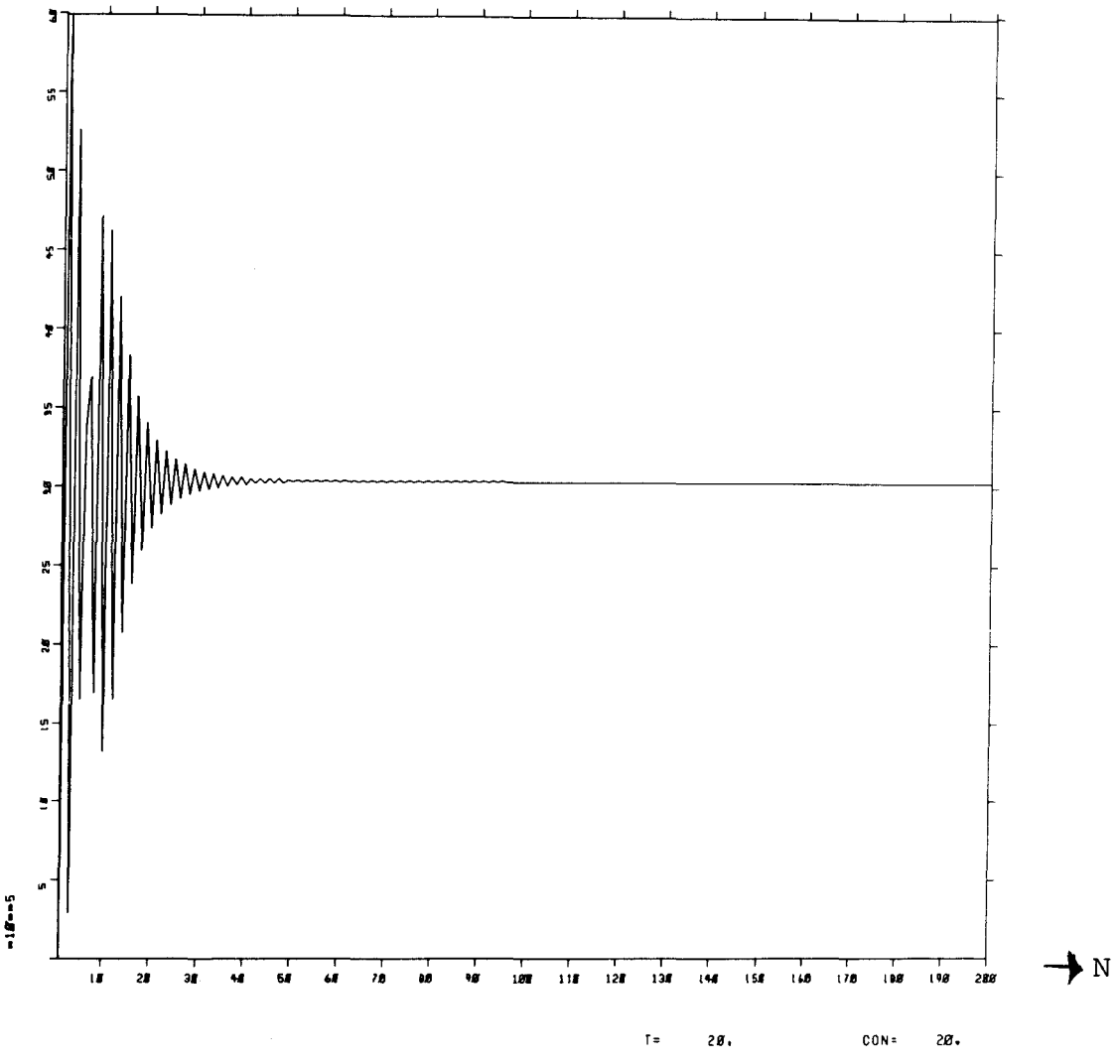

Fig. 5

are always equal to one.

That means $f_N(2o)$ with CON=18/2o has no 'step' causing misleading results (compare Fig. 5).

The auxiliary quantities $f_N(1oo)$ and $f_N(18o)$ with CON=5 (necessary for the computation of the discretization error) have steps at N=2o and N=55 (compare Fig. 6 and Fig. 7).

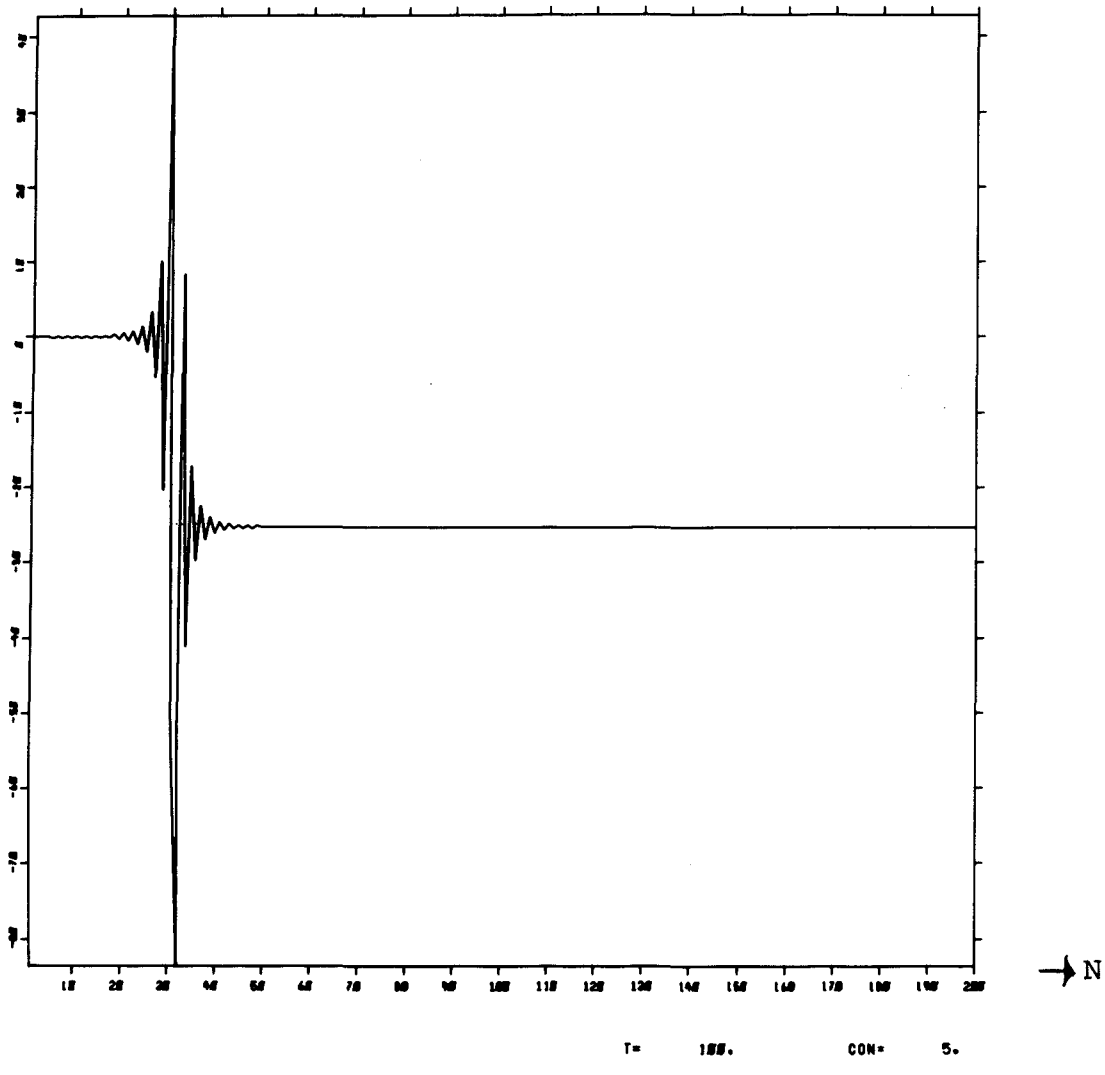

Fig. 6

Hence the control digit for $f_N(1oo)$ has to be zero if NS1$\leq$6o , and the one for $f_N(18o)$ if NS1$\leq$165 . This coincides with the results listed in Table 7.

It follows that CON_{OPT} and the error computed by (33) are accurate only for NS1>165 if the ε-algorithm is used. The MINIMAX-method leads to an accurate error estimation already for NS1>55 (see Table 7).

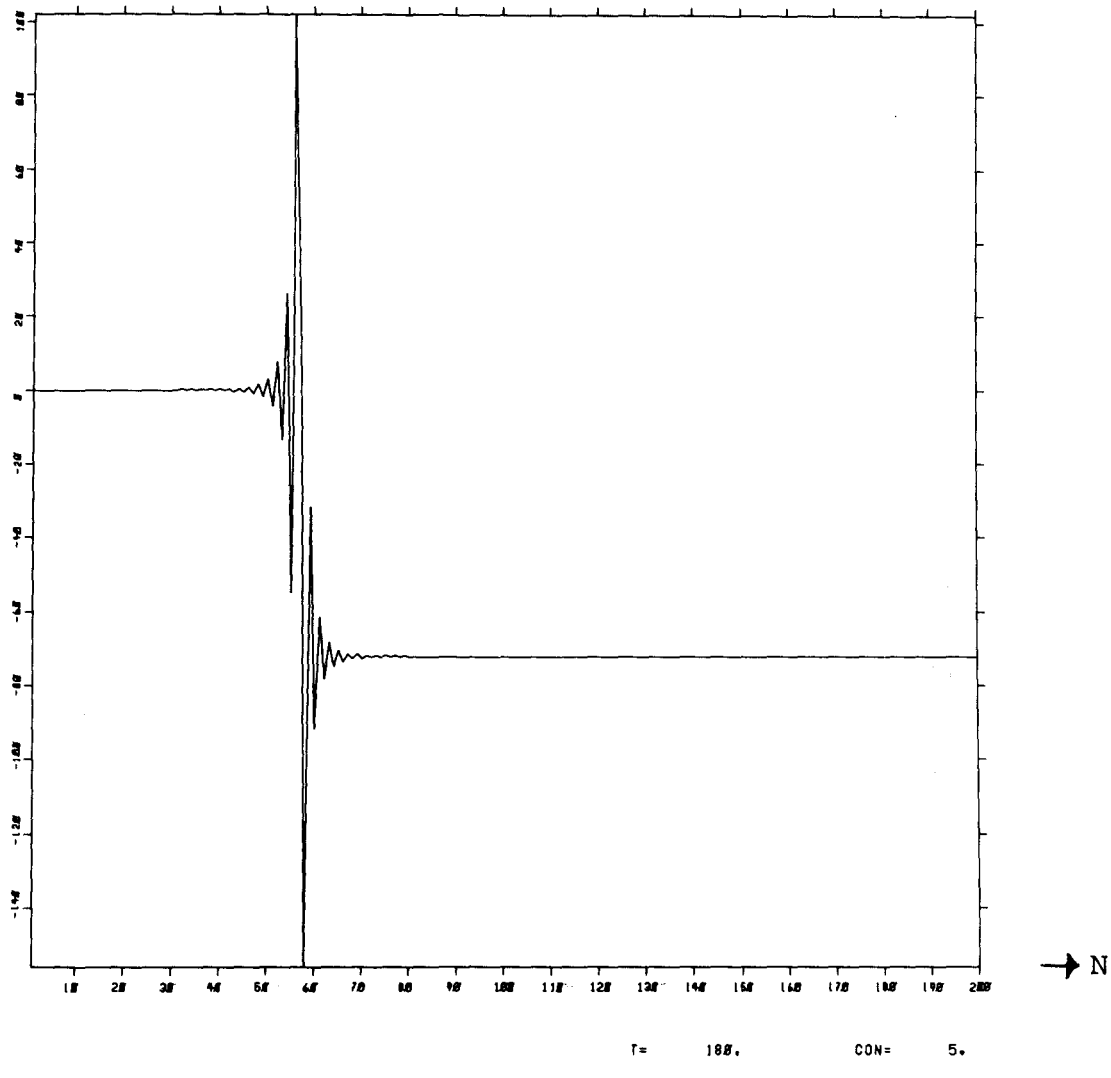

Fig. 7

The control digit referring to $f_N(2o)$ with $CON=CON_{OPT}=4.3$ is equal to one (see Tab. 7). Hence no falsification of the results occurs for the given values of NS1 (see Fig. 8). The "Korrektur"-term $f_N(6o)$ with $CON=CON_{OPT}$, however, has a control digit that is equal to two if $NS2 \leq 2o$ and $NS2 \geq 6o$, equal to zero otherwise. Hence a 'step' must occur at $N=2o$.

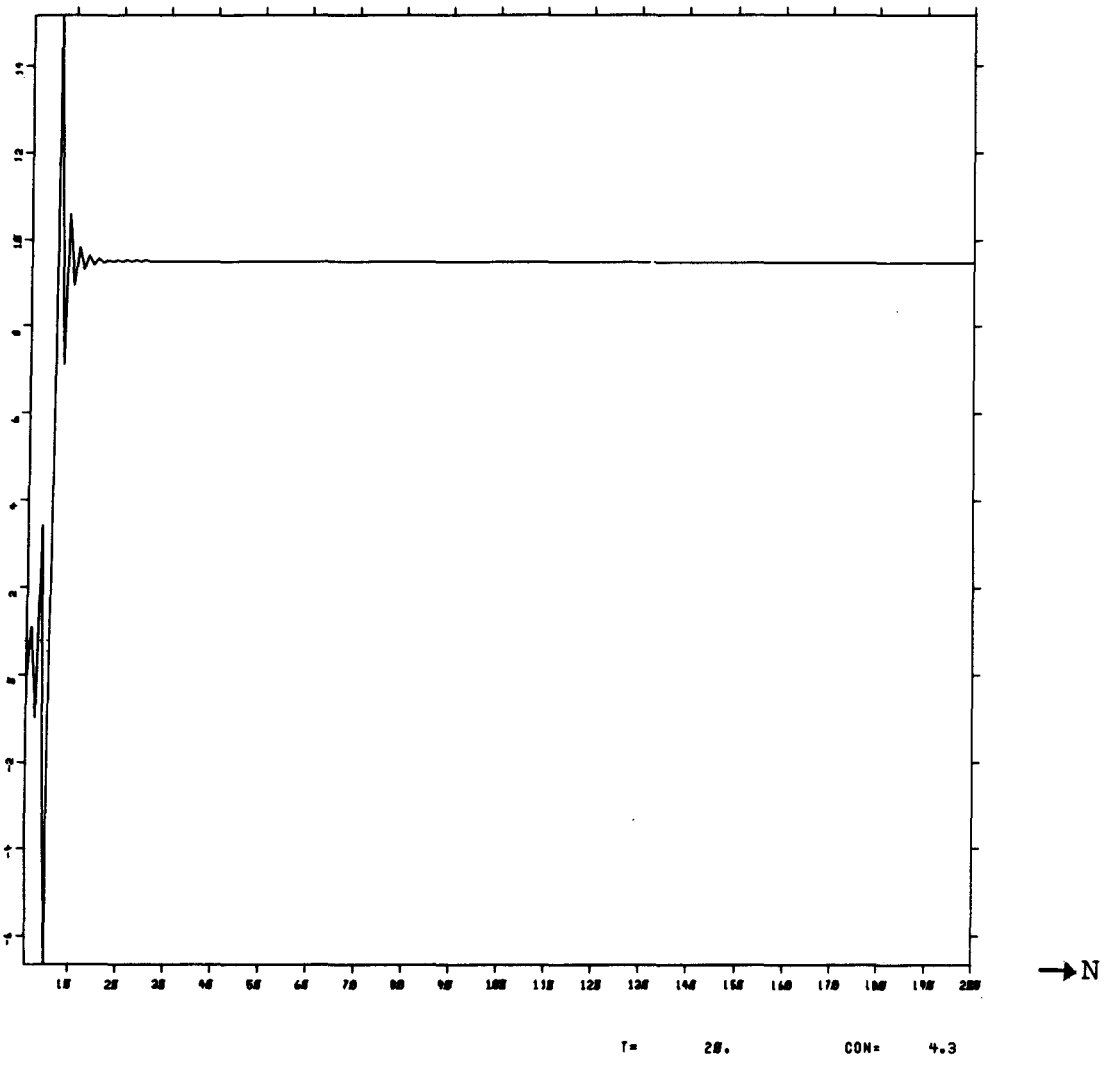

Fig. 8

This is confirmed by Fig. 9. Therefore the error in Table 7 is large for NS2=1o and NS2=2o and of course the error computed by (33) doesn't coincide with the real error for these values of NS2 . We can conclude: in the above example the results computed by LAPIN are accurate for NS1>55 and

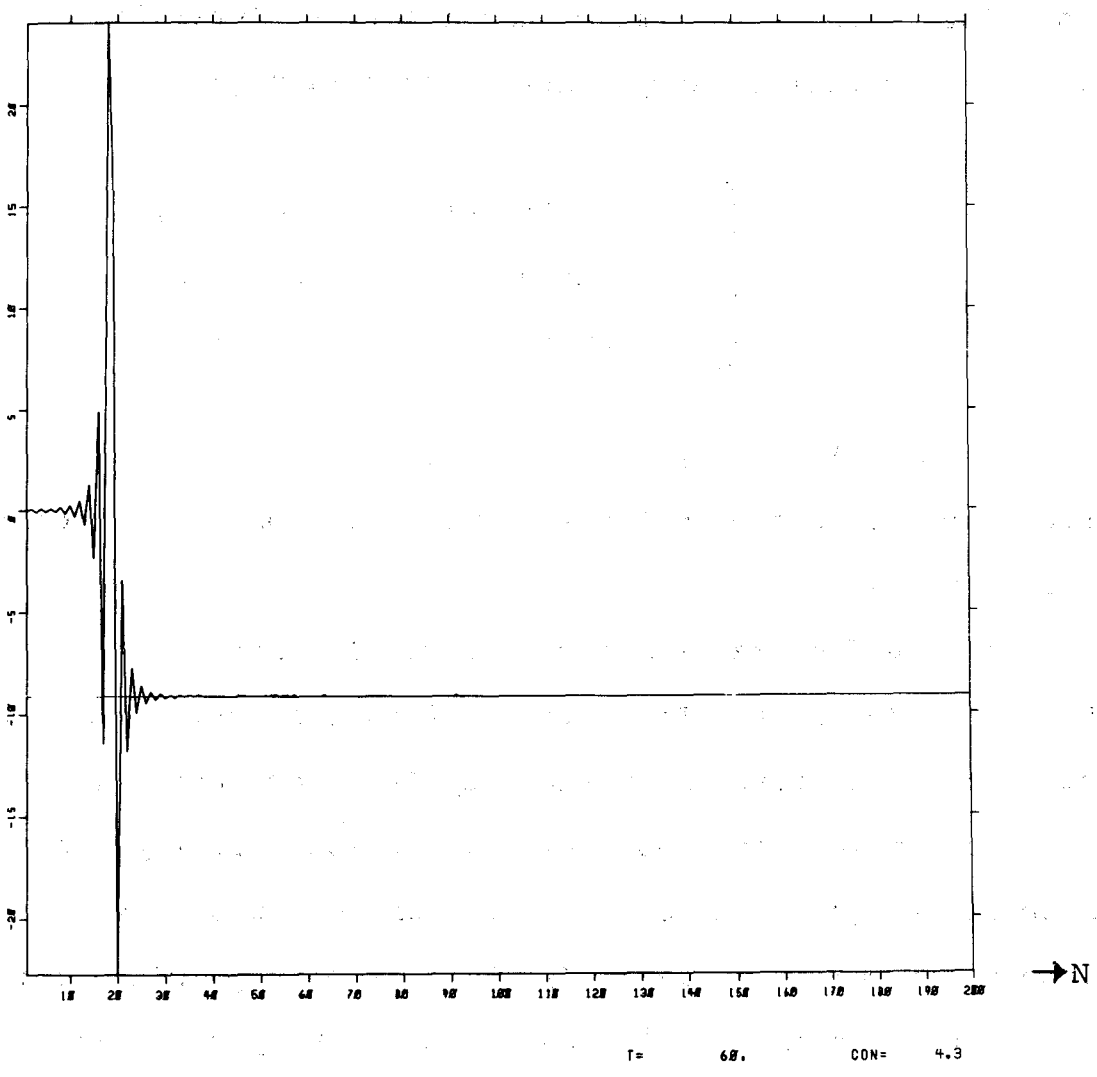

Fig. 9

NS2>2o if MINIMAX is used; this holds for the ε-algorithm not until NS1>165 and NS2>6o . It should be mentioned again that in the case the MINIMAX-method is accurate but the ε-algorithm is not, LAPIN always uses MINIMAX to accelerate the convergence of the series and that this is indicated by the corresponding control digit (by a zero).

As a last example we discuss the numerical inversion of the Laplace transformed step function (see also [5]):

$$f^{st}(t) = \begin{cases} 2 & 2n<t<2(n+1)\ , \quad n=o,2,4,... \\ 1 & t=2n\ , \quad n=o,1,2,3,... \\ o & 2n<t<2(n+1)\ ; \quad n=1,3,5,... \end{cases}$$

$(F(s) = L[f(t)] = 2/\{s(1+\exp(-2s))\}\ )$

From Table 8 we see that the accuracy is low at the points $t=2n\ ,\ n=o,1,2,...$

A similar effect was already observed inverting $F(s) = \exp(-1os)/s$. The inverse of this function has a step at $t=1o$. The results obtained by LAPIN got worse if t was close to $t=1o$ (see Table 4). With a sufficiently large NS1 , however, we got good results even for t-values close to $t=1o$ (see right column of Table 4). This is also possible for $F(s) = 2/\{s(1+\exp(-2s))\}$. The high accuracy we achieved with LAPIN at the step $t=1o$ for $F(s) = \exp(-1os)/s$ is not attainable here because $f_N^{st}(2n)\ ,\ n=o,1,2,...$ is not monotonous in N and hence the curve fitting method (CFM) is not applicable.

The diminished accuracy close to a step of the original function $f(t)$ can be explained by the behaviour of $f_N(t)$ as a function of N . Fig. 1o shows $f_N(t)$ $(f(t) = L^{-1}[\exp(-1os)/s])$ for $t = 9.6$(A) ; 9.7(B) ; 9.8(C) , Fig. 11 for $t = 9.8$(A) ; 9.9(B) ; 9.94(C) ; 9.96(D); 1o.o(E).

$f(t) = f^{st}(t)$; $F(s) = 2/\{s(1+\exp(-2s))\}$

method code	LAPIN 1 - 1 - o - 2 NS1=2oo
	absolute error
t 1	o.488 D-11
2	o.23o D-o2
3	o.714 D-o8
4	o.997 D-o2
5	o.3o2 D-11
6	o.742 D-o3
7	o.714 D-o8
8	o.4o6 D-o2
9	o.217 D-1o
1o	o.226 D-o2
CPU-time	3.91 sec(for t=1(1)2o)

Table 8

It is obvious that the number of stationary values of $f_N(t)$ in a fixed interval $o \leq N \leq N_o$ is smaller the closer t is to t=1o . Hence the convergence of the Fourier series is slow - even if it is accelerated with EPAL or MINIMAX.

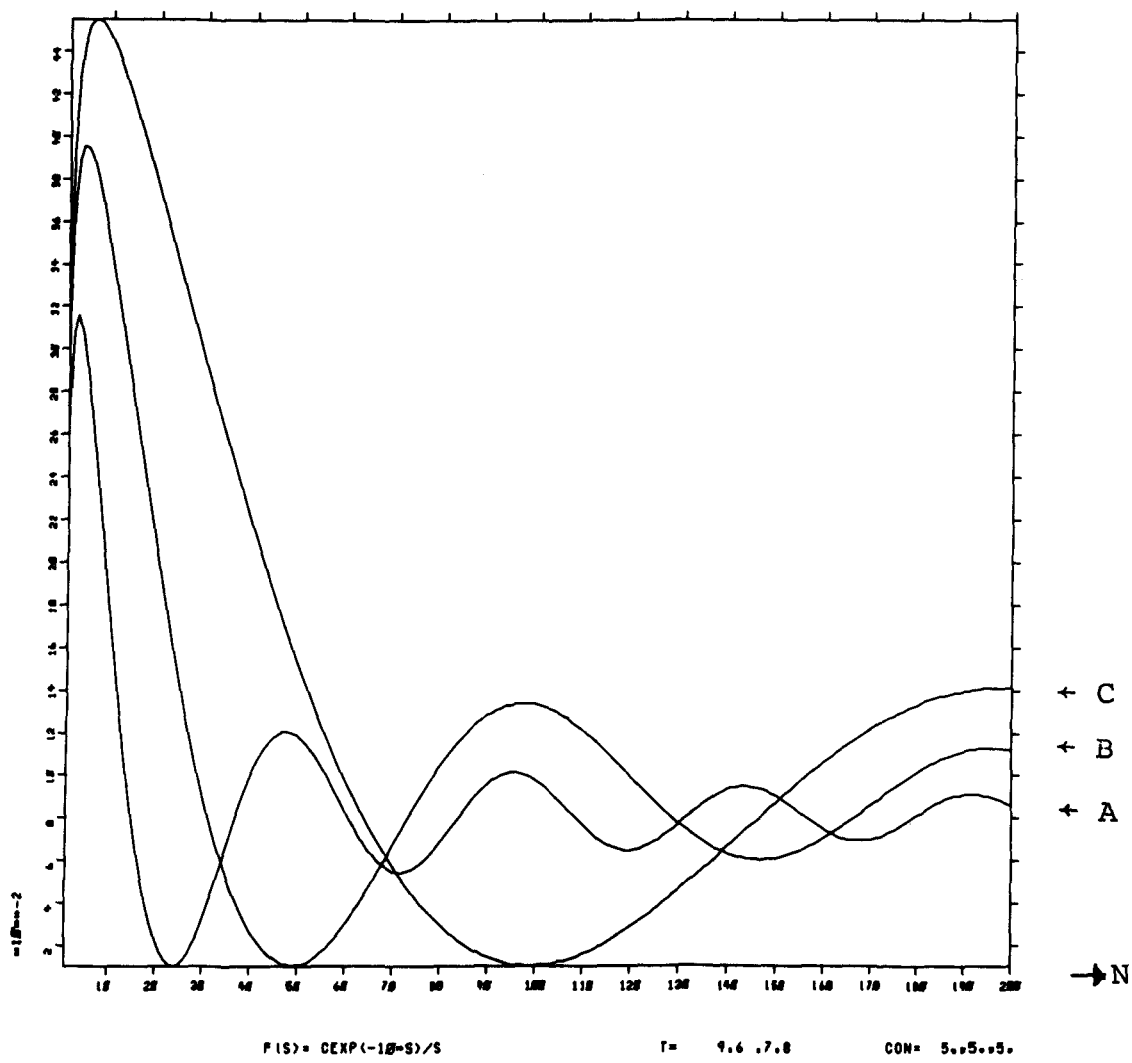

Fig. 1o

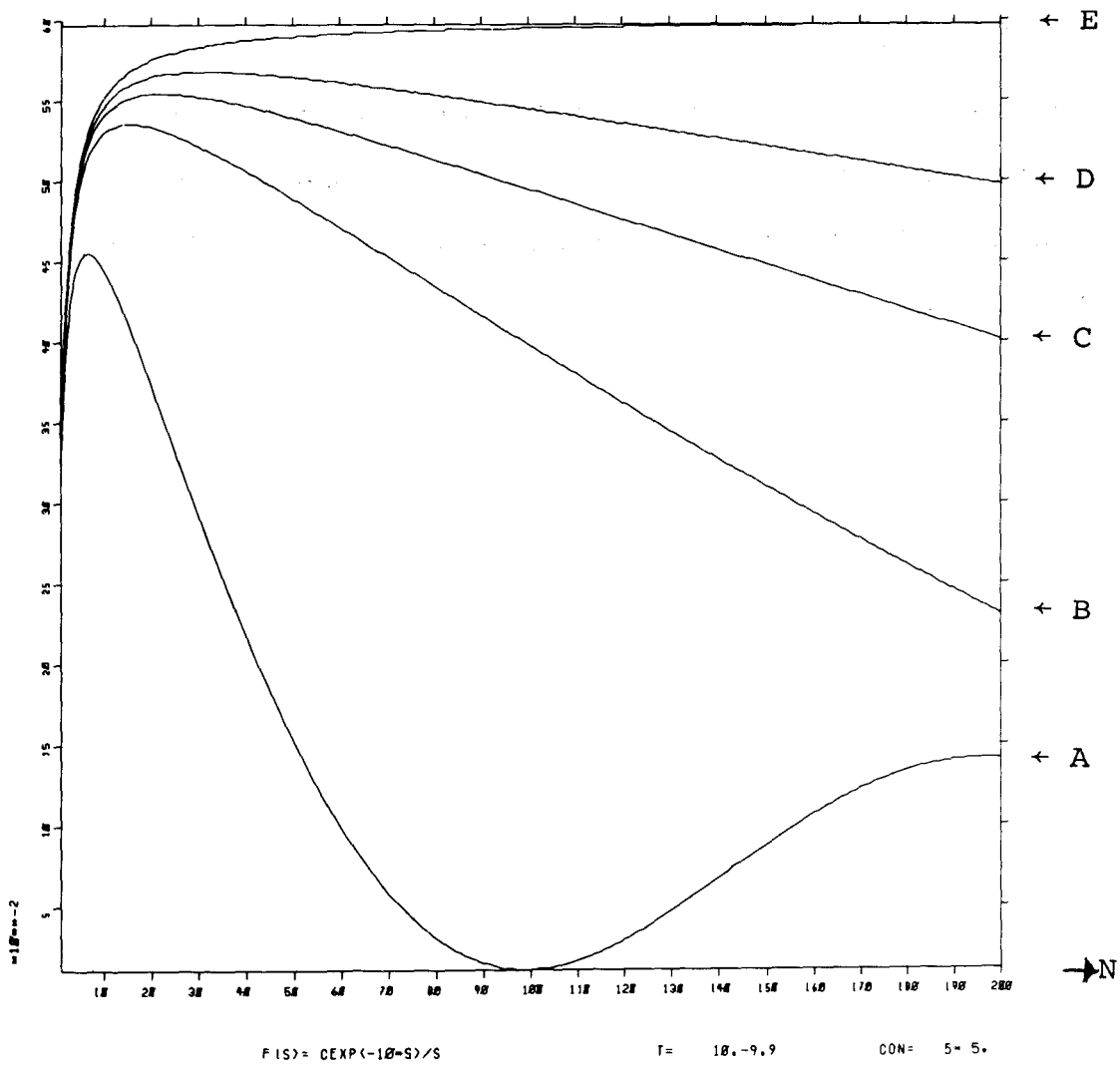

Fig. 11

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A P P E N D I X

```
      SUBROUTINE LAPIN(F,T1,TN,N,IMAN,ILAPIN,IKONV,NS1,NS2,ICON,
     *                 IKOR,CON,H,E,IER)
C
      IMPLICIT REAL*8(A-H,O-Z)
      COMPLEX*16 F,FUNC
      INTEGER*4 RICHT,RICHTA,HMONO
      EXTERNAL F
      DIMENSION H(6,N),E(3,NS1),E3(3)
C
C     CALL MASKE
      IER = 0
      IF (TN.LT.T1) IER = 1
      IF (N.LT.1) IER = IER+10
      I = IMAN+1
      GO TO (100,110),I
      IER = IER+100
      GO TO 120
C
C PARAMETERS FOR IMAN = 0
  100 IF (NS1.NE.60) IER = IER+10000
      IF (IER.NE.0) GO TO 120
      ILAPIN = 1
      IKONV = 2
      ICON = 1
      IKOR = 0
      NS2 = 0
      GO TO 200
C
C IMAN = 1
  110 IF (ILAPIN.LT.1 .OR. ILAPIN.GT.2) IER = IER+1000
      IF (IKONV.LT.1 .OR. IKONV.GT.2) IER = IER+10000
      IF (NS1.LT.1 .OR. (NS2.LT.1 .AND. IKOR.EQ.1)) IER = IER+100000
      IF (ICON.LT.0 .OR. ICON.GT.2 .OR. (ICON.EQ.2 .AND. ILAPIN.EQ.2))
     *   IER = IER+1000000
      IF (IKOR.LT.0 .OR. IKOR.GT.1) IER = IER+10000000
      IF (ICON.EQ.0.AND.CON.LE.0.D0) IER = IER+100000000
      IF (IER.EQ.0) GO TO 200
  120 WRITE(6,1) IER,T1,TN,N,IMAN,ILAPIN,IKONV,NS1,NS2,ICON,IKOR,CON
    1 FORMAT(///' *** ERROR ***',8X,'IER =',I12//
     * ' T1      | ',D10.3,18X,'1 |  TN < T1'/
     * ' TN      | ',D10.3/
     * ' N       | ',I10,17X,'10 |  N < 1'/
     * ' IMAN    | ',I10,16X,'100 |  IMAN < 0  OR  IMAN > 1'/
     * ' ILAPIN  | ',I10,15X,'1000 |  ILAPIN < 1  OR  ILAPIN > 2'/
     * ' IKONV   | ',I10,14X,'10000 |  IKONV < 1  OR  IKONV > 2'/
     * ' NS1     | ',I10,13X,'100000 |  NS1 < 1  OR  (NS2 < 1  AND  ',
     *                              'IKOR = 1)'/
     * ' NS2     | ',I10/
     * ' ICON    | ',I10,12X,'1000000 |  ICON < 0  OR ICON > 2  OR',
     *                               '  (ICON = 2  AND  ILAPIN = 2)'/
     * ' IKOR    | ',I10,11X,'10000000 |  IKOR < 0  OR  IKOR > 1'/
     * ' CON     | ',D10.3,10X,'100000000 |  CON <= 0'//)
      RETURN
C
  200 PI = 4.D0*DATAN(1.D0)
      CON1 = 20.D0
      CON2 = CON1-2.D0
      ABSF = 0.D0
C
      J3 = (3-ICON)/2+N*(ICON/2)
      TA = T1
      TB = TN
C
      DO 830 L3=1,J3
      HMONO = 0
      KOR1 = IKOR
C
C COMPUTATION OF THE OPTIMAL PARAMETERS
  210 IF (ICON-1) 360,230,220
  220 TA = T1+L3*(TN-T1)/(N+1)
      TB = TA
```

```
C
  230 NH = N/2
      T = TA+(TB-TA)*NH/(N+1)
      TK = (2-ILAPIN)*T+(ILAPIN-1)*TB
C
C COMPUTATION OF THE TRUNCATION ERROR (RNSUM)
      TO = T
      CON = CON1
      JUMP = 1
      GO TO 370
  240 FN = H(1,L3)
      FNS1 = E(1,NS1)
      CON = CON2
      JUMP = 2
      GO TO 370
  250 IF (FN.NE.H(1,L3).AND.FNS1.NE.E(1,NS1)) GO TO 255
      CONOPT = CON
      ABSF = 0.D0
      GO TO 320
  255 RNSUM = TK*(FN-H(1,L3))/(DEXP(CON1)-DEXP(CON2))
      IF (ILAPIN.EQ.2) GO TO 260
C
C COMPUTATION OF THE ACCELERATION FACTOR (DEL)
      RACC = T*(FNS1-E(1,NS1))/(DEXP(CON1)-DEXP(CON2))
      DEL = RNSUM/RACC
C
  260 IF (IKOR.EQ.1) GO TO 280
C
C OPTIMAL PARAMETERS (METHOD A)
      TO = 2.D0*TK+T
      CON = CON1/4.D0
      JUMP = 3
      GO TO 370
  270 FN = H(1,L3)
      CONOPT = -TK/(2.D0*TK+T)*DLOG(DABS(RNSUM/(TK*FN)))
      GO TO 310
C
C OPTIMAL PARAMETERS FOR THE KORREKTUR METHOD (METHOD A)
  280 TO = 4.D0*TK+T
      CON = CON1/4.D0
      JUMP = 4
      GO TO 370
  290 FN = H(1,L3)
      TO = 8.D0*TK+T
      JUMP = 5
      GO TO 370
  300 FN = FN-H(1,L3)
      CONOPT = -TK/(4.D0*TK+T)*DLOG(DABS(RNSUM/(TK*FN)))
C
C OPTIMAL PARAMETERS (METHOD B)
  310 IF (ILAPIN.EQ.1) GO TO 315
      ABSF = DABS(DEXP(CONOPT)*RNSUM*2.D0/TK)
      GO TO 320
  315 V1 = CON1/T
      V2 = CONOPT/T
      EINS = 1.D0
      IF (NS1/2*2.NE.NS1) EINS = -1.D0
      RNSUMK = RNSUM*(DREAL(F(DCMPLX(V2,PI*NS1/T)))*EINS)/
     *                (DREAL(F(DCMPLX(V1,PI*NS1/T)))*EINS)
      ABRN = (RNSUMK-RNSUM)/(V2-V1)
      CONOPT = -DLOG(DABS((ABRN/T+RNSUMK)/(T*(IKOR*2+2)*FN)))/
     *          (3.D0+2.D0*IKOR)
      V1 = V2
      V2 = CONOPT/T
      RNSUMK = RNSUMK*(DREAL(F(DCMPLX(V2,PI*NS1/T)))*EINS)/
     *                (DREAL(F(DCMPLX(V1,PI*NS1/T)))*EINS)
      ABSF = DEXP(CONOPT)/T*DABS(RNSUMK)+
     *       DABS(DEXP(-2.D0*CONOPT)*FN*(IKOR-1)
     *           +DEXP(-4.D0*CONOPT)*FN*IKOR)
C
  320 IF (CONOPT.LE.0.D0) CONOPT = 1.D0
C
```

```
C LAPLACE-INVERSION WITH OPTIMAL PARAMETERS
C
      TO = TA
      TT = TB
      I1 = L3
      J1 = (2-ICON)*N+(ICON-1)*L3
      CON = CONOPT
      KOR1 = IKOR
      JUMP = 6
      GO TO 380
C
  360 TO = T1
      TT = TN
      I1 = 1
      J1 = N
      KOR1 = IKOR
      JUMP = 6
      GO TO 380
C
  370 KOR1 = 0
      TT = TO
      I1 = L3
      J1 = L3
C
  380 DELTA = (TT-TO)/DFLOAT(N+1)
      K2 = 1
      NSUM = NS1
C
C COMPUTATION OF THE T-VALUES FROM TO,TT
  400 IF (ILAPIN.EQ.1) GO TO 420
      TE = K2*TT
      V = CON/TE
      RAL = -0.5D0*DREAL(F(DCMPLX(V,0.D0)))
      PITE = PI/TE
C
  405 DO 410 L=1,NSUM
      W = (L-1)*PITE
      FUNC = F(DCMPLX(V,W))
      E(2,L) = DREAL(FUNC)
      E(3,L) = DIMAG(FUNC)
  410 CONTINUE
C
  420 DO 800 K1=I1,J1
C
      TL = TO+K1*DELTA
      IF (ILAPIN.EQ.2) GO TO 440
C
      IF (K2.EQ.2) TL = 3.D0*TL
      V = CON/TL
      FAKTOR  =  DEXP(V*TL)/TL
      RAL = -0.5D0*DREAL(F(DCMPLX(V,0.D0)))
      PIT = PI/TL
      EINS = 1.D0
      SURE = 0.D0
C
C METHOD OF DURBIN
  425 DO 430 L=1,NSUM
      W = (L-1)*PIT
      SURE = SURE+DREAL(F(DCMPLX(V,W)))*EINS
      EINS = -EINS
      E(1,L) = FAKTOR*(RAL+SURE)
  430 CONTINUE
      GO TO 460
C
  440 IF (K2.EQ.2) TL = TL+TE
      FAKTOR = DEXP(V*TL)/TE
      SURE = 0.D0
      SUIM = 0.D0
      DO 450 L=1,NSUM
      W = (L-1)*PITE
      SURE = SURE+E(2,L)*DCOS(W*TL)
      SUIM = SUIM+E(3,L)*DSIN(W*TL)
```

```
      E(1,L) = FAKTOR*(RAL+SURE-SUM)
  450 CONTINUE
C
C SEARCH FOR STATIONARY VALUES
  460 NMAX = NSUM*2/3
      MONOTO = 0
      K = 0
      RICHTA = DSIGN(1.5D0,(E(1,NSUM)-E(1,NSUM-1)))
      DO 500 L=1,NMAX
      J = NSUM-L
      RICHT = DSIGN(1.5D0,(E(1,J)-E(1,J-1)))
      IF (RICHT.EQ.RICHTA) GO TO 500
      K = K+1
      E3(K) = E(1,J)
      IF (K.EQ.3) GO TO 510
      RICHTA = RICHT
  500 CONTINUE
      IF (K.EQ.0) GO TO 700
      H(K2,K1) = E(1,NSUM)
      IF (K2.EQ.1) H(4,K1) = 0
      GO TO 790
  510 KE = 1
  520 RICHTA = RICHT
      KE = 3-KE
      IF ((E3(KE)-E(1,J))*RICHTA.GT.0.D0) GO TO 560
  540 IF (J.LE.NSUM/3) GO TO 550
      J = J-1
      RICHT = DSIGN(1.5D0,(E(1,J)-E(1,J-1)))
      IF (RICHT-RICHTA) 520,540,520
  550 MONOTO = 1
      IF (IKONV.EQ.2) GO TO 630
C
C MINIMUM-MAXIMUM METHOD (MINIMAX)
  560 H(K2,K1) = (E3(1)+E3(3))/4.D0+E3(2)/2.D0
      IF (K2.EQ.1) H(4,K1) = 1
      GO TO 790
C
C EPSILONALGORITHM (EPAL)
  630 K = 0
      NSUMM1 = NSUM-1
      E2 = E(1,1)
      DO 660 L=1,NSUMM1
      E1 = E(1,1)
      TM = 0.D0
      LP1 = L+1
      DO 650 M=1,L
      MM = LP1-M
      TM1 = E(1,MM)
      DIVI = E(1,MM+1)-E(1,MM)
      IF (DABS(DIVI).GT.1.D-20) GO TO 640
      K = L
      GO TO 670
  640 E(1,MM) = TM+1.D0/DIVI
      TM = TM1
  650 CONTINUE
      E2 = E1
  660 CONTINUE
C
  670 IF (DABS(E1).GT.DABS(E2)) E1 = E2
      IF(DABS(E(1,1)).GT.DABS(E1)) E(1,1) = E1
      H(K2,K1) = E(1,1)
      IF (K2.EQ.1) H(4,K1) = K+2
      GO TO 790
C
C CURVE FITTING (CFM)
  700 X1 = NSUM-2.D0
      X2 = NSUM-1.D0
      X3 = NSUM-0.D0
      Y1 = E(1,NSUM-2)
      Y2 = E(1,NSUM-1)
      Y3 = E(1,NSUM)
      B = ((Y3-Y1)*X3*X3*(X1+X2)/(X1-X3)
```

```
     *     -(Y2-Y1)*X2*X2*(X1+X3)/(X1-X2))/(X3-X2)
           A = ((Y2-Y1)-B*(X1-X2)/(X1*X2))*(X2*X2*X1*X1)/(X1*X1-X2*X2)
           H(K2,K1) = Y1-(A/X1+B)/X1
           MONOTO = 1
           IF (K2.EQ.1) H(4,K1) = 3
C
C
  790 H(3,K1) = CON
           H(5,K1) = ABSF
           HMONO = HMONO+K2*MONOTO*10**(6-JUMP)
           IF (JUMP.LT.6) GO TO 800
           H(6,K1) = (2-K2)*HMONO+(K2-1)*(2*MONOTO+H(6,K1))
           HMONO = HMONO/10*10
C
  800 CONTINUE
           IF (KOR1.EQ.0) GO TO (240,250,270,290,300,830),JUMP
           IF (K2.EQ.2) GO TO 810
           K2 = 2
           NSUM = NS2
           GO TO 400
C
C KORREKTUR METHOD
  810 FAKTOR = -DEXP(-2.D0*CON)
           DO 820 K=I1,J1
           H(1,K) = H(1,K)+FAKTOR*H(2,K)
  820 CONTINUE
C
           GO TO (240,250,270,290,300,830),JUMP
  830 CONTINUE
           RETURN
           END
```