On the Accurate Computation of Singular Solutions of Laplace’s and Poisson’s Equation

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ABSTRACT

 Singularities in the solution destroy the accuracy of numerical approximations to elliptic problems. Unfortunately due to a pollution effect the accuracy deteriorates globally in the whole domain. On equidistant meshes certain corrections can be used in order to recover the high accuracy. In particular the polluting effect can be suppressed.

 These corrections are studied for interesting model situations like Laplace’s equation with nonsmooth boundary data and Poisson’s equation with singular source terms. Theoretical as well as experimental results demonstrate that $h^2$ convergence as for smooth solutions is obtained.

 The application of the corrections within the multigrid method is discussed. In particular the combination with Richardson or $\tau$-extrapolation is shown to allow the highly accurate computation of singular solutions.

1. Introduction.

 Typical error estimates for the numerical solution of boundary value problems depend on the smoothness of the true solution. In many error estimates norms of the solution derivatives play an essential role. Elliptic boundary value problems may have singular solutions, however. The solution has unbounded derivatives (or is itself unbounded) in the neighborhood of certain points of the solution domain. Such singularities may be caused by a variety of situations, which happen to be present in many practical applications. Reasons for the emergence of singularities can for example be reentrant corners, discontinuous coefficients, source terms with singularities (i.e. point loads, dipoles, etc.) or singular functions in the boundary conditions.

 Singularities in the solution can cause difficult numerical problems. If no precautions are taken, the accuracy deteriorates depending on the strength of the singularity. Problems with discontinuous coefficients may locally behave
like $r^a$, where $r$ is the distance from the singularity and the exponent is $a=0.1$ or worse. In this case the error expansion starts with terms $h^{a}$. This rate of convergence is unacceptably slow. Additionally there is the so called pollution effect. The deterioration in accuracy is not restricted to a neighborhood of the singularity but the accuracy is destroyed in the whole domain.

Furthermore, iterative solvers for the discrete equations may become less efficient. This has also been observed in the multigrid method. If the discrete solutions are poor approximations to the true solutions, coarse grid solutions are poor approximations to fine grid solutions. Thus the coarse grid correction process in a multigrid method is less effective.

One technique for avoiding above problems is to use local grid refinement. Though this is the standard approach, it has some obvious disadvantages. The data structures get much more complex, making implementation difficult. The computational overhead for processing these data structures may be quite large.

So there is the question whether simple modifications of the discrete equations on equidistant grids can recover satisfactory accuracy. For the case of reentrant corners such modifications have been suggested in [12] and [4]. The situation with discontinuous coefficients has been examined in [8]. In all these situations $O(h^a)$ accuracy could be recovered. The difference equations were modified at a single point of the regular grid, only.

This paper is concerned with the remaining cases: Explicit singularities in the boundary conditions and singularities in the source terms. We suggest to use equidistant grids with modifications of the boundary values (respectively source terms) only. We will show analytically and experimentally that $O(h^a)$ convergence can be recovered at points far from the singularity. The pollution effect is eliminated. For the case of singular boundary conditions it will even be shown that the modification of one boundary value is sufficient for getting $O(h^a)$ convergence.

For simplicity we will study Laplace's and Poisson's equation on rectangular two-dimensional domains, only. The basic idea, however, is not restricted to these simple model problems. It can be extended to more general regions and operators. Our results are formulated for the case of one isolated singularity in the solution domain. Of course they can be generalized to cases with several singularities by using the superposition principle.

The paper is organized as follows. Section 2 introduces some notation and cites two theorems on which our technique is based.

The third section studies solutions with singularities in the boundary conditions. Two theorems show that $O(h^a)$ convergence can be obtained by either smoothing the boundary values in a fixed neighborhood of the singularity or, alternatively, modifying one single boundary value. These theoretical results are certified by numerical experiments. Richardson’s extrapolation may be used to improve the accuracy further.

In the fourth section we examine Poisson’s equation when the source terms are point loads or derivatives of delta functions. One problem is to define numerical equivalents of these unbounded source terms. It will be shown that if the correct numerical analogue are chosen, the order of convergence is $O(h^a)$.

The fifth section is devoted to $\tau$-extrapolation. This is a multigrid specific extrapolation technique. It is usually also based on smoothness assumptions on the true solution. We will demonstrate that it can also used for singular solutions. In this case the type of singularity and corresponding error expansions must be considered when choosing the extrapolation parameters. As another alternative $\tau$-extrapolation may be combined with the modifications introduced earlier, leading to very accurate approximations.

2. Basic Definitions and Theorems

In this section we introduce some basic notation and results. The Laplace operator $\Delta$ in two dimensions is defined by

$$\Delta = \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right]$$

For studying difference equations we introduce the difference operators

$$d_x u(x,y) = h^a \left[ u(x-h,y) - 2u(x,y) + u(x+h,y) \right]$$
$$d_y u(x,y) = h^a \left[ u(x,y-h) - 2u(x,y) + u(x,y+h) \right]$$

The usual 5-point discretization $\Delta_h$ of the Laplace operator is defined by

$$\Delta_h = \frac{d_x^2 + d_y^2}{2}$$

In this paper we restrict our attention to the unit square

$$\Omega = (0,1) \times (0,1)$$

$\overline{\Omega}$ denotes the closure and $\partial \Omega$ the boundary of $\Omega$. The numerical approximations are defined on equidistant grids with meshsize $h$:

$$\Omega_h = \left\{ (ih,jh), 0 \leq i,j \leq N, h=1/N, i,j \text{ integer} \right\}$$

$\overline{\Omega}_h$ is defined by

$$\overline{\Omega}_h = \left\{ (ih,jh), 0 \leq i,j \leq N, h=1/N, i,j \text{ integer} \right\}$$

and the boundary of $\Omega_h$ by

$$\partial \Omega_h = \overline{\Omega}_h - \Omega_h$$
The following definition and theorem is taken from [12].

**Definition:** A family of functions \( u_h(x,y) \) is called \( h \)-bounded on \( \Omega \), if there exists a real-valued, continuous function \( r(x,y) \) on \( \Omega \) (not necessarily bounded on \( \Omega \)), such that for every \((x,y)\in\Omega\) there exists \( h_r > 0 \), such that \[ |u_h(x,y)| < r(x,y) \text{ for all } h < h_r, \quad h = 1/N, \quad N \text{ integer, } (x,y)\in\Omega. \] If \( r(x,y) \) is bounded on \( \Omega \), \( u_h(x,y) \) is called strictly \( h \)-bounded.

The crucial point about \( h \)-boundedness is that a \( h \)-bounded family of grid-functions \( u_h(x,y) \) may be unbounded on \( \Omega \) for \( h>0 \), but because of the continuity of \( r(x,y) \) it is bounded on any compact subset of \( \Omega \), for all \( h \). This definition is used in

**Theorem 2.1:**

Let the solution of

\[ \Delta u = f \quad \text{on } \Omega, \]

be bounded on \( \bar{\Omega} \). If \( \frac{d^2 u}{dx^2} + \frac{d^2 u}{dy^2} = f \) is \( h \)-bounded on \( \Omega \) for \( \delta \in (0,1) \) and \( \delta \in (0,1) \), then:

\[ \delta^2 \frac{d^2 u}{dx^2} f \quad \text{is } h \text{-bounded on } \Omega. \]

The proof is given in [12].

Asymptotic error expansions for the Laplace equation in rectangular domains are studied in [5]. Even when there are singularities on the boundary, the existence of asymptotic expansions can be proved. We present one result in

**Theorem 2.2:**

Let \( u^s \) be the solution of the boundary value problem

\[ \Delta u = 0 \quad \text{in } \Omega, \]

\[ u = f(x) \quad \text{on } \partial \Omega, \quad y=0, \]

\[ u = 0 \quad \text{on } \partial \Omega, \quad y=\neq 0, \]

where \( f(x) \) has a singularity at the point \((x_0,0)\in\partial \Omega_1:\)

\[ f(x) = \left[ g(x) \cdot (x-x_0)^p \right], \quad a>0, \]

with an analytic function \( g(x) \) on \((0,1)\). Let \( u_\delta \) be the numerical solution

\[ \Delta u_\delta = 0 \quad \text{in } \Omega, \]

\[ u_\delta = f(x) \quad \text{on } \partial \Omega, \quad y=0, \]

\[ u_\delta = 0 \quad \text{on } \partial \Omega, \quad y=\neq 0. \]

Then, there exists an asymptotic expansion

\[ u_\delta = u^s + \sum_{n=1}^{\infty} \delta^n u_{\delta n} + \sum_{n=1}^{\infty} \delta^n u_{\delta n}, \]

For the proof see [8].

3. Singularities in the boundary conditions.

In this section we study situations as described in theorem 2.2, in some more detail. For these problems the analytically correct solution \( u^s \) contains singular components:

\[ u^s(x,y) = \text{Im} \left[ g(x+iy) \cdot (x-x_0+iy)^p \right] + \text{smooth terms}, \quad a>0, \quad x_0 \in (0,1), \]

with \( g(x) \) analytic on the closure of \( \Omega \). \( u^s(x,y) \) is harmonic in \( \Omega \). Provided \( u^s \) additionally satisfies the boundary conditions it must be the correct solution. \( u^s \) has unbounded derivatives on \( \partial \Omega \). No theorem based on the smoothness of the true solution is applicable. There are general results giving convergence orders for the corresponding finite difference solutions. For example \( O(h^3) \) accuracy is guaranteed by the theorems in [2]. However, if the singularity is located on the boundary, the situation is not that bad. Hohmann's theory (see theorem 2.2 and [6]) shows that the numerical solution \( u_\delta \) has an asymptotic expansion starting with a term of order \( O(h^3) \) at fixed points in the interior of \( \Omega \) if \( 0<\delta<1 \). The essential ideas of Hohmann's proof are also used in theorem 3.3 below.

With the following theorems we demonstrate that \( O(h^3) \) convergence (as for smooth solutions) can be recovered, if the boundary values \( f(x,y) \) are modified to \( f_\delta(x,y) \). This convergence rate is valid only for fixed points in \( \Omega \), not for points approaching the singularity, when \( h \to 0 \). The first theorem is based on studying a related, smooth problem.

**Theorem 3.1:**

Let \( u^s \) be the solution of the boundary value problem

\[ \Delta u = 0 \quad \text{in } \Omega, \]

\[ u = f(x,y) \quad \text{on } \partial \Omega, \]

where \( f(x,y) \) has a singularity at \((x_0,0)\in\partial \Omega_1:\)

\[ f(x,y) = \text{Im} \left[ g(x+iy) \cdot (x-x_0+iy)^p \right], \quad a>0, \]

with \( g(x) \) analytic on \( \bar{\Omega}, \quad 0<\delta<1 \). (Under these conditions \( f(x,y) \) defines a harmonic function on \( \Omega \) satisfying the boundary conditions and thus \( u^s(x,y) = f(x,y) \)). Let \( u_\delta \) be the solution of the modified numerical analogue

\[ \Delta u_\delta = 0 \quad \text{in } \Omega, \]

\[ u_\delta = f_\delta(x,y) \quad \text{on } \partial \Omega, \quad y=0, \]

\[ u_\delta = 0 \quad \text{on } \partial \Omega, \quad y=\neq 0, \]

where \( F(x,y) \) is a function satisfying
\[ \frac{\partial}{\partial t} F(x,y) = f(x,y), \]

Then:
\[ u_b = u^* + h^2 R_b, \]

where \( R_b \) is \( h \)-bounded on \( \Omega \).

**Proof:** Consider the related problem
\[ \Delta U = 0 \quad \text{in} \; \Omega, \]
\[ U = F(x,y) \quad \text{on} \; \partial \Omega, \]

with the exact solution \( U^* \) (\( \frac{\partial^2}{\partial x^2} U^* = u^* \)) and the numerical analogue
\[ \Delta_b U_b = 0 \quad \text{in} \; \Omega_b, \]
\[ U_b = F(x,y) \quad \text{on} \; \partial \Omega_b, \]

If \( R_b \) is defined by
\[ U_b = U^* + h^2 R_b, \]

then
\[ \Delta_b R_b = \frac{1}{h^2} \Delta_b U^* \quad \text{in} \; \Omega_b, \]
\[ R_b = 0 \quad \text{on} \; \partial \Omega_b. \]

The right hand side of this problem satisfies
\[ 1. \quad -\frac{1}{h^2} \Delta_b U^* \text{ is } h \text{-bounded in } \Omega, \]
\[ 2. \quad \frac{1}{h^2} \left[ \frac{\partial^2}{\partial x^2} U^* \right] \text{ is } h \text{-bounded in } \Omega. \]

This can be seen by using Taylor expansions and smoothness properties of \( U^* \) for estimating the remainder terms. Furthermore \( R_b \) is bounded on \( \bar{\Omega}_b \) (see e.g. [6]).

Using theorem 2.1 this implies that \( \frac{\partial^2}{\partial y^2} R_b \) is \( h \)-bounded in \( \Omega \).

Now define \( \tilde{U}_b = \frac{\partial^2}{\partial y^2} U_b \). (\( U_b \) can be extended to points outside \( \Omega_b \) such that \( \Delta_b U_b = 0 \) at points on the boundary, and thus \( \tilde{U}_b \) is defined in \( \bar{\Omega}_b \) including the boundary.) \( \tilde{U}_b \) is the solution of a finite difference equation
\[ \Delta_b \tilde{U}_b = 0 \quad \text{in} \; \Omega_b, \]
\[ \tilde{U}_b = \frac{\partial^2}{\partial y^2} F(x,y) \quad \text{on horizontal boundary lines}, \]
\[ \tilde{U}_b = \frac{\partial^2}{\partial y^2} F(x,y) + O(h^2) \quad \text{on vertical boundary lines}. \]

Moreover
\[ \Delta_b u^* = \frac{\partial^2}{\partial y^2} \left[ U_b - U^* \right] + \left[ \frac{\partial^2}{\partial x^2} U_b - \frac{\partial^2}{\partial x^2} U^* \right] = h^2 \left[ \frac{\partial^2}{\partial y^2} q_b + q_b \right]. \]

Both \( \frac{\partial^2}{\partial y^2} q_b \) and \( q_b \) term are \( h \)-bounded on \( \Omega \).

It remains to show that \( \tilde{U}_b - u_b \) is of order \( O(h^3) \). This, however, can be easily seen by comparing the corresponding numerical boundary value problems. They differ only in the boundary values, and this difference is of order \( O(h^3) \). The discrete maximum principle guarantees that \( \tilde{U}_b - u_b \) is \( h \)-bounded gridfunction. This completes the proof. \( \Box \)

**Remark:** Theorem 3.1 can be sharpened to
\[ u_b = u^* + h^2 u_b + O(h^3) \]

using the more involved techniques of the following theorem.

Note that the modification of the boundary values to \( \tilde{F} \) need only be done in a fixed neighborhood of the singularity. A suitable \( \tilde{F} \) can be constructed using one of the following formulas
\[ \tilde{F}(x) = \int_{x-a \cdot h}^{x + a \cdot h} f(t) dt \]

or equivalently
\[ \tilde{F}(x) = \int_{-h}^{h} K(x, h) f(t) dt, \]

where the kernel \( K(x, h) \) is given by
\[ K(x, h) = \begin{cases} \frac{h - |x|}{h^2} & \text{for } |x| < h \\ 0 & \text{otherwise} \end{cases} \]

This procedure is a smoothing of the boundary values. The integral kernel is a linear B-spline. If B-splines of higher order are used, the boundary values are smoothed more. Then \( h^3 \) expansions of the error up to corresponding orders can be obtained.

In the following we will discuss an alternative technique and proof. This approach will lead to one point modifications. It is interesting that it is possible to obtain the improvement in convergence by modifying not all values along a boundary line, but at a single point only. This time the proof is based on explicit representations of the true and numerical solution as Fourier series. Our result is stated in
Theorem 3.3:
Let $u^*$ be the solution of the boundary value problem

$$\Delta u = 0 \quad \text{in} \quad \Omega,$$

$$u = f(x) \quad \text{on} \quad \partial \Omega, \quad y > 0,$$

$$u = 0 \quad \text{on} \quad \partial \Omega, \quad y = 0,$$

where $f(x)$ has a singularity at $x_0 \in (0,1)$, $x_0 = \text{M}h$, $M$ integer:

$$f(x) = \begin{cases} g(x)(x-x_0)^\alpha & \text{for} \quad x < x_0, \\ 0 & \text{otherwise.} \end{cases}$$

Assume that $g(x)$ is analytic on $[x_0, 1]$ and $0 < \alpha < 2$. Let $u_h$ be the solution of the modified numerical analogue

$$\Delta_h u_h = 0 \quad \text{in} \quad \Omega_h,$$

$$u_h = f(x) \quad \text{on} \quad \partial \Omega_h, \quad y > 0,$$

$$u_h = 0 \quad \text{on} \quad \partial \Omega_h, \quad y = 0.$$

Here $f(x)$ is defined by

$$\tilde{f}(x) = \begin{cases} -h^\alpha g(x_0) \zeta(\alpha) & \text{for} \quad x < x_0, \\ f(x) & \text{otherwise,} \end{cases}$$

where $\zeta$ is Riemann’s $\zeta$-function.

Then $u_h$ has an asymptotic expansion

$$u_h = u^* + h^\alpha u_1 + O(h^{2\alpha}).$$

Proof: According to Hofmann [6] the true solution and the numerical solution can be represented by

$$u(x,y) = \sum_{n=1}^\infty a_n \sin(n\pi x) T(n,y) \quad \text{for} \quad y > 0$$

and

$$u_h(x,y) = \sum_{n=1}^{\infty} b_n(N) \sin(n\pi x) T(n,y) \quad \text{for} \quad y > 0$$

respectively, $h = 1/N$. $T(n,y)$ is defined by

$$T(n,y) = \frac{\sinh(n\pi(1-y))}{\sinh(n\pi)}$$

The numbers $a_n$ are Fourier coefficients

$$a_n = 2 \int_0^1 f(x) \sin(n\pi x) \, dx.$$

The numbers $b_n(N)$ are trapezoidal sums

$$b_n(N) = \frac{2}{N} \sum_{i=1}^{N-1} f\left(\frac{i}{N}\right) \sin\left(\frac{n\pi i}{N}\right)$$

and $\mu_\alpha$ is defined by the equation

$$\sinh\left(\frac{\mu_\alpha}{2N}\right) = \sin\left(\frac{\alpha\pi}{2N}\right).$$

Following [6] the discretization error can be split into three terms.

$$u^*(x,y) - u_h(x,y) = I_1(x,y,h) + I_2(x,y,h) + I_3(x,y,h)$$

where

$$I_1(x,y,h) = \sum_{n=1}^\infty a_n \sin(n\pi x) T(n,y),$$

$$I_2(x,y,h) = \sum_{n=1}^{\infty} a_n \sin(n\pi x) \left[ T(n,y) - T(\mu_\alpha, y) \right],$$

$$I_3(x,y,h) = \sum_{n=1}^\infty (a_n - b_n(N)) \sin(n\pi x) T(\mu_\alpha, y).$$

The first two terms have asymptotic expansions in terms of $h^\alpha$ if $f(x)$ is bounded, piecewise continuous, and satisfies

$$f(x) = \frac{1}{2} \left( \lim_{i \to 0} f(x+i) + \lim_{i \to T} f(x+i) \right) \quad \text{for} \quad 0 < \chi < 1$$

$$f(0) = \lim_{x \to 0} f(x)$$

$$f(1) = \lim_{x \to 1} f(x).$$

In contrast, $I_2$ depends on further properties of $f$. In the above representation of $I_2$ the numerical integration error

$$a_n - b_n(N) = 2 \left( \int_0^1 f(x) \sin(n\pi x) \, dx - \frac{1}{N} \sum_{i=1}^{N-1} f\left(\frac{i}{N}\right) \sin\left(\frac{n\pi i}{N}\right) \right)$$

play an essential role.

In fact, Hofmann proves that if the numerical integration error of the first Fourier coefficient has an error expansion of the form

$$a_1 - b_1(N) = \sum_{i=1}^\infty \beta_i h^i + O(h^{\alpha+1})$$
then \( I_1 \) (and thus the discretisation error) can be expanded to
\[
\begin{align*}
u(x,y) - u_0(x,y) &= \sum_{i=1}^{r} s_i(x,y) h^{m+1} + O(h^{m+1})
\end{align*}
\]
where the \( s_i \) are members of the finite set of numbers
\[
\{2j+i, j \geq 0, i \geq 0, 2j+i \leq \gamma_p\}
\]

Thus the problem reduces to determining the error of a numerical integration. We can use a result of [11], which gives a generalisation of the Euler–Maclaurin formula. If \( f(x) \) is analytic in \( 0 < x < 1, \alpha > 0 \) then
\[
\begin{align*}
\int_0^1 x^n f(x) \, dx &= \frac{1}{N} \sum_{k=1}^{N} \left( \frac{k}{N} \right)^n f \left( \frac{k}{N} \right) + \frac{B_n}{2} f(0) + O(h^{m+1})
\end{align*}
\]
where \( B_n \) are Bernoulli numbers. Using \( x_0 = \frac{N}{h} \)
\[
\begin{align*}
a_0 - b_0(N) &= 2 \int_0^1 f(x) \sin(n \pi x) \, dx - \frac{1}{N} \sum_{i=1}^{N} f \left( \frac{i}{N} \right) \sin \left( \frac{N i}{N} - \frac{1}{N} f(x_0) \sin(n \pi x_0) \right)
\end{align*}
\]

Numerical experiments.

Now we demonstrate the effectiveness of our techniques with numerical experiments. The test problem is
\[
\begin{align*}
\Delta u &= 0 \quad \text{on } \Omega,
\end{align*}
\]
\[
\begin{align*}
u(x,y) = \Re \left( (x+i(y-0.5))^{1.5} \right) \quad \text{on } \partial \Omega,
\end{align*}
\]
such that the analytically correct solution is
\[
\begin{align*}
u(x,y) = \Re \left( (x+i(y-0.5))^{1.5} \right) = x^2 \cos(\varphi/2),
\end{align*}
\]
where
\[
\begin{align*}r = |x+i(y-0.5)|, \quad \varphi = \arg(x+i(y-0.5)).
\end{align*}
\]
This function is shown in the figure below.

Figure 1.

We compare three different numerical methods. Method 1 uses the unmodified boundary conditions. Here the results of Hofmann predict $O(h^{10})$ convergence. For Method 2 the boundary values are replaced by smoothed ones according to theorems 3.1. Method 3 finally uses a single modification at the point (0.5,0) according to theorem 3.2. In particular $f(1,2,0) = \varphi_{(-0.5)-1}h^n = 0.207886h^{10}$ replaces $f(1,2,0) = 0$. The calculations are performed on grids with $h = 1/8, 1/16, 1/32, 1/64, 1/128$. The following table shows the discretization errors $\varepsilon(x,y) - \varepsilon(x,y)$ evaluated at points $(x,y)\in\Omega$. The last column gives the average convergence order.

<table>
<thead>
<tr>
<th>$(x,y)$</th>
<th>meshsize (h)</th>
<th>1/8</th>
<th>1/16</th>
<th>1/32</th>
<th>1/64</th>
<th>1/128</th>
<th>conv. order</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(1/2,1/2)$</td>
<td>1</td>
<td>.101e-1</td>
<td>.324e-2</td>
<td>.108e-2</td>
<td>.369e-3</td>
<td>.127e-3</td>
<td>1.58</td>
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<td>2</td>
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<td>.212e-3</td>
<td>.552e-4</td>
<td>.132e-4</td>
<td>.336e-5</td>
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<tr>
<td>3</td>
<td>.209e-2</td>
<td>.495e-3</td>
<td>.122e-3</td>
<td>.305e-4</td>
<td>.763e-5</td>
<td>2.02</td>
<td></td>
</tr>
<tr>
<td>$(1/4,1/2)$</td>
<td>1</td>
<td>.636e-2</td>
<td>.214e-2</td>
<td>.720e-3</td>
<td>.244e-3</td>
<td>.837e-4</td>
<td>1.56</td>
</tr>
<tr>
<td>2</td>
<td>.639e-3</td>
<td>.174e-3</td>
<td>.447e-4</td>
<td>.112e-4</td>
<td>.281e-5</td>
<td>1.95</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>.150e-2</td>
<td>.402e-3</td>
<td>.103e-3</td>
<td>.253e-4</td>
<td>.664e-5</td>
<td>1.95</td>
<td></td>
</tr>
<tr>
<td>$(1/8,h)$</td>
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<td>.462e-1</td>
<td>.326e-1</td>
<td>.233e-1</td>
<td>.164e-1</td>
<td>0.48</td>
</tr>
<tr>
<td>2</td>
<td>.543e-3</td>
<td>.121e-3</td>
<td>.808e-4</td>
<td>.558e-4</td>
<td>.393e-4</td>
<td>0.65</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>.121e-1</td>
<td>.874e-2</td>
<td>.618e-2</td>
<td>.437e-2</td>
<td>.309e-2</td>
<td>0.49</td>
<td></td>
</tr>
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</table>

At the point in the interior of the domain the predicted convergence orders can be clearly observed. Method 2 and 3 both converge with $O(h^{10})$, though method 2 yields somewhat lower errors. Method 1 demonstrates the pollution effect. Even far from the singularity the convergence deteriorates to $O(h^{10})$. Further note that at the point approaching the singularity all methods converge with $O(h^{10})$ only.

Richardson extrapolation can be used on these results. In method 1 the $O(h^{10})$ errors can be eliminated, in method 2 and 3 the $O(h^{10})$ errors. For integrating Richardson’s extrapolation into a full multigrid algorithm see [10]. The following table presents the results. The last column gives the average convergence order of the extrapolated results.

<table>
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<td>$(1/2,1/2)$</td>
<td>1</td>
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</tr>
<tr>
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<td>-.527e-6</td>
<td>-.867e-7</td>
<td>2.91</td>
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</tr>
</tbody>
</table>

- 13 -
4. Point loads and higher derivatives of delta functions.

Singular solutions can also be caused by the equation's right hand side. An especially interesting case are point loads, that is source terms which contain delta functions (or their derivatives). When trying to solve such a problem numerically, the first question is how to model the unbounded delta function. At this point a similar trick as in the previous section is used. The numerical equivalent of the delta function is obtained by integrating the original delta function and taking the corresponding finite differences of the result. This is an analogous smoothing operation as was used in the previous section. The following theorem gives the detail.

We start with a definition. The (generalized) functions $H_i$ ($i$ integer) are defined by

$$H_i(x) = \begin{cases} 
0 & \text{for } x < 0 \\
\frac{1}{2} & \text{for } x = 0 \\
1 & \text{for } x > 0 
\end{cases}$$

and recursively

$$H_i(x) = \left\{ \begin{array}{ll}
\frac{d}{dx} H_{i-1}(x) & \text{for } i > 0 \\
\int \limits_{-\infty}^{x} H_{i-1}(\xi) d\xi & \text{for } i < 0
\end{array} \right.$$ 

Derivatives are to be understood in the distributional sense. Note that $H_0$ is the Heaviside step function and $H_1$ is the Dirac-$\delta$-function.

**Theorem 4.1:**

Let $u^*$ be the (weak) solution of the boundary value problem

$$\Delta u = H_\mu(x-x_0)H_\nu(y-y_0) \quad \text{in } \Omega$$

$$u = 0 \quad \text{on } \partial \Omega$$

where $\mu, \nu$ are positive integers and $(x_0, y_0) \in \Omega$. Let $u_\delta$ be the solution of

$$\Delta_\delta u_\delta = f_\delta \quad \text{in } \Omega_\delta$$

$$u_\delta = 0 \quad \text{on } \partial \Omega_\delta$$

where

$$f_\delta = d_\delta^m d_\delta^n \left[H_{\mu-2\delta}(x-x_0)H_{\nu-2\delta}(y-y_0)\right]$$

and where $m, n, \delta$ are chosen such that $2m, 2n, \delta$ and $H_{\mu-2\delta}(x-x_0)H_{\nu-2\delta}(y-y_0)$ are continuous functions.

Then:

$$u_\delta = u^* + h^\delta \chi_\delta$$

where $\chi_\delta$ is $h$-bounded on $\Omega - \{(x_0, y_0)\}$.

**Proof:**

Smooth boundary values (in the rectangle) cause errors with $h^\delta$ expansions. Thus we may change the boundary values (of the differential and numerical problem) to

$$u_\delta(x, y) = g(x, y) \quad \text{on } \partial \Omega$$

where

$$g(x, y) = \frac{1}{2\pi} \frac{2^\mu-1}{2^\nu-1} \ln \left[ \left((x-x_0)^2 + (y-y_0)^2\right)^{1/n} \right]$$

The solution is given by

$$u^*(x, y) = g(x, y)$$

We study the 'integrated' problem

$$\Delta U = H_{\mu-2\delta}(x-x_0)H_{\nu-2\delta}(y-y_0) \quad \text{in } \Omega$$

$$U = F(x, y) \quad \text{on } \partial \Omega$$

where

$$\frac{2^\mu-1}{2^\nu-1} F(x, y) = g(x, y)$$

and its numerical equivalent

$$\Delta_\delta U_\delta = H_{\mu-2\delta}(x-x_0)H_{\nu-2\delta}(y-y_0) \quad \text{in } \Omega_\delta$$

$$U_\delta = F(x, y) \quad \text{on } \partial \Omega_\delta$$

Define $R_\delta$ by

$$U_\delta = u^* + h^\delta R_\delta$$

$R_\delta$ satisfies

$$\Delta_\delta R_\delta = \delta_\delta - \frac{1}{h^\delta} \left[H_{\mu-2\delta}(x-x_0)H_{\nu-2\delta}(y-y_0) - \Delta_\delta u^*\right]$$

Using Taylor-expansions and smoothness properties of $U^*$ for estimating the remainder terms we can show that

1. $R_\delta$ is bounded on $\Omega_\delta$.
2. $d_\delta^m d_\delta^n R_\delta$ is $h$-bounded on $\Omega - \{(x_0, y_0)\}$ for all $0 < k \leq m$ and $0 < l \leq n$.

Because of these two properties $R_\delta$ is bounded on $\Omega$. Now we define

$$\delta_\delta := d_\delta^m d_\delta^n U_\delta \text{ on } \Omega_\delta$$
where the necessary values of \( U_h \) outside \( \Omega_h \) are assumed such that \( U_h \) satisfies \( \Delta_h \tilde{U}_h = P(x,y) \) on the boundary of \( \Omega_h \) (and sufficiently many points outside \( \Omega_h \)), too. \( \tilde{U}_h \) satisfies
\[
\Delta_h \tilde{U}_h = f_h \quad \text{on} \quad \Omega_h
\]
\[
\tilde{U}_h = g(x,y) + h^3 F_h \quad \text{on} \quad \partial \Omega_h
\]
where (because of the smoothness of \( u \) along the boundary) \( F_h \) is \( h \)-bounded.
Thus \( u_h \) and \( \tilde{U}_h \) are solutions to almost the same numerical boundary value problem, and, because of the discrete maximum principle cannot differ by more than order \( O(h^3) \). Furthermore
\[
\tilde{U}_h = d_h^u \partial_h^3 U_h + h^3 \partial_h^3 R_h = u_h + \left( d_h^u \partial_h^3 U_h - u_h \right) + h^3 \partial_h^3 R_h
\]
Now \( d_h^u \partial_h^3 U_h - u_h \) and \( h^3 \partial_h^3 R_h \) are \( h \)-bounded on \( \Omega - \{(x_0,y_0)\} \). This proves the theorem. \( \Box \)

Numerical example.

We give a numerical example. The test problem is as in theorem 4.1, with a point load, i.e. \( \mu = 1 \). In the numerical equivalent the right hand side is given by
\[
f_h(x,y) = \begin{cases} 0 & \text{for } |x-x_0| > h \text{ or } |y-y_0| > h \\ \frac{(h-|x-x_0|)(h-|y-y_0|)}{h^4} & \text{for } |x-x_0| < h \text{ and } |y-y_0| < h \end{cases}
\]
This is equivalent to
\[
f_h(x,y) = d_h^u \partial_h^3 H_h(x-x_0) H_h(y-y_0)
\]
In the example we use \((x_0,y_0) = (1/3,1/3)\). Note that this is no meshpoint. The boundary values are chosen correspondingly, as in the proof of theorem 4.1, so that the true solution of the example is given by
\[
u_h(x,y) = \frac{1}{2\pi} \ln \left| \frac{(x-1/3)^2 + (y-1/3)^2}{(x-1/3)^2 + (y-1/3)^2} \right|
\]
The table summarizes experimental results for this problem. For different values of \( h \) we measure the error at fixed points inside the region \( R \).

<table>
<thead>
<tr>
<th>Discretization Errors for Point Loads</th>
</tr>
</thead>
<tbody>
<tr>
<td>point</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>meshsize</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

The predicted \( O(h^3) \) convergence behavior can be observed for \( h < 1/16 \).

5. \( \tau \)-extrapolation in the presence of singularities.

A very interesting technique for improving the accuracy of solutions in the multigrid method is the so-called \( \tau \)-extrapolation. In this section we will discuss how \( \tau \)-extrapolation can be used in the presence of singularities.

In a regular multigrid algorithm two iterations are used alternatingly. The smoother:
\[
u_h^{(k)} = u_h + S(f_h-L_h u_h)
\]
and the coarse grid correction (for a two grid method):
\[
u_h^{(k+1)} = u_h^{(k)} + \frac{1}{2} L_h^2 u_h^{(k)}(f_h-L_h u_h)
\]
These two iterations have a common fixed point described by \( f_h-L_h u_h = 0 \).

The typical efficiency of multigrid as a solver of the fixed point equation is caused by the different convergence properties. The smoother converges fast for certain (usually the high frequency) solution components, but converges only slowly for the remaining (low frequency) modes. In contrast the coarse grid correction converges fast for the low frequency modes, but diverges (slowly) for the high frequency components. If these contrary properties combine the usual multigrid efficiency is obtained. In this consideration multigrid is viewed only as a solver for a discrete system of equations. The accuracy of the solution with respect to the solution of the differential problem is only related to the discretization of \( L \). In this perspective multigrid has no effect on the accuracy of the numerical solution with respect to the analytical solution. Certain properties of the analytical solution, like the presence of singularities, may of course have effects on the accuracy of the multigrid solver.

The multigrid technique, however, also offers algorithmic possibilities to improve not only the algebraic convergence (convergence towards the discrete solution \( u_h \)) but also the differential convergence (the accuracy of \( u_h \) with respect to the analytically correct solution).
The different convergence properties imply that high frequency solution modes in the discrete solution are mainly supplied by the smoothing process, while low frequency components are contributed by the coarse grid correction. On the other hand, consistency is a property of low frequency modes. This leads to the idea of double discretization: in the coarse grid correction process higher order discretizations may be used. Because of the above considerations one may hope that the final solution accuracy is improved despite the smoother being applied with respect to the old, less accurate discretizations. This is the basic idea of double discretization. It can also be understood as a special, multigrid specific, defect correction technique. A rigorous analysis can be found in [1] and [5].

$\tau$-extrapolation, finally is a special defect correction (double discretization) technique. The coarse grid correction is changed to

$$u^{(c)} = u^{(c)*} + h^2 L_L^2 u^{(c)*} + (1 - \gamma) (L_L^2 u^{(c)*} + L_L^2 u^{(c)*}) + \gamma L_L^2 (L_L^2 u^{(c)*} + L_L^2 u^{(c)*})$$

The defect $L_L^2 u^{(c)}$ is replaced by a linear combination of defects of different grid levels. A high order difference scheme is constructed by combining the low order difference operators on different grids.

This differs from a standard truncation error extrapolation by still using smoothing with respect to the old, low order equations. Two iterative processes having different fixed points are applied. This may cause problems. Details can be found in [3,9].

Assume the true solution is sufficiently smooth and the truncation errors have asymptotic expansions in terms of $h^4$. If the restrictions $L_L^2$ are chosen appropriately, the linear combination of defects with $1 = 4/3$ will be of order $O(h^4)$. Further assuming that the multi-grid iteration converges with a contraction rate independent of $h$, one can show that the limit of the method cannot differ from the true solution by more than $O(h^4)$. For this one must observe that a standard smoother like Gauss-Seidel changes smooth solutions only by $O(h^4)$.

All these considerations depend on the smoothness of the true solution. The improvement in accuracy must be expected to fail in the presence of singularities. In the following we will present experimental results showing that $\tau$-extrapolation may still be used, even when the solution has singularities. However, one must either apply modifications as introduced above, or use extrapolation parameters adapted to the special asymptotic behavior.

Numerical example.

We demonstrate the effectiveness of $\tau$-extrapolation with a numerical experiment. The example is

$$\Delta u = 0 \quad \text{on } \Omega$$

$$u = \Re \left( (x + iy)^{-1/2} \right)^{1/4} \text{ on } \partial \Omega$$

The true solution is depicted in the following figure.

![Figure 2.](image)

We compare several approaches. The problem is first discretised and solved without modification. This is method 1. For method 2 we use a $\tau$-extrapolation where the extrapolation parameter is chosen such that possible $h^4$ terms in the defect are eliminated. In the third variant a similar extrapolation is performed. But here the parameter is chosen such that order $h^{14}$ terms are eliminated. The last two experiments combine the corrections of section 3 with $\tau$-extrapolation. Experiment 4 gives the results for a solution with modifications as described in theorem 3.1 but uses no extrapolation yet. The 5th experiment uses the same, modified boundary values, but finally applies an additional $\tau$-extrapolation eliminating $h^4$ terms. The table gives the results. The error is again measured at fixed points of the domain. The last column gives the average convergence order.
Errors for Variants of Multigrid Methods with $\tau$-Extrapolation

<table>
<thead>
<tr>
<th>meshsize $(x,y)$</th>
<th>method</th>
<th>1/8</th>
<th>1/16</th>
<th>1/32</th>
<th>1/64</th>
<th>1/128 conv.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>order</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(1/2,1/2)</td>
<td>1</td>
<td>-3.88e-2</td>
<td>-1.51e-2</td>
<td>-5.18e-3</td>
<td>-2.56e-3</td>
<td>-1.07e-3</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>-1.87e-2</td>
<td>-7.35e-3</td>
<td>-3.20e-3</td>
<td>-1.35e-3</td>
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<td>4.74e-3</td>
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<td>1.36e-5</td>
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<tr>
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<td>4</td>
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<td>-2.07e-5</td>
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<td>(1/2,h)</td>
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<td>-1.79e-3</td>
<td>-1.51e-3</td>
<td>-1.27e-3</td>
<td>-1.07e-3</td>
</tr>
</tbody>
</table>

Note the following observations:

1. The normal method shows $O(h^{16})$ convergence.
2. So does the method with $\tau$-extrapolation of $O(h^4)$ terms. Here only the absolute size of the errors is improved by a factor, not the order of convergence.
3. When the extrapolation is performed with respect to $O(h^{14})$ then the convergence behavior is improved to $O(h^4)$.
4. A quite similar accuracy (better by a constant factor) is obtained with a completely different technique: modification of the boundary values and straightforward solution of the discrete system.
5. If these modifications are combined with $\tau$-extrapolation of $h^4$ errors the results are (experimentally) $O(h^4)$ accurate.
6. In the immediate neighborhood of the singularity all methods converge with order $h^{16}$ only. The absolute error, however, is improved by the boundary modifications.
7. Note that corrections combined with extrapolation yield better accuracy with meshsize $h=1/8$ than the standard approach with $h=1/128$. Or, seen from the other side, in order to get errors like $10^{-4}$ with the standard algorithms, one would need meshes as fine as $h=1/10^4$. This is far beyond what can presently be treated by any method.

Note that not all convergence results are justified by the theory of the previous sections. We never proved the existence of $h$ expansions up to order $h^6$. Additionally there is the problem that $\tau$-extrapolation does not improve the solution directly. Its influence is indirect and based on the truncation errors. A more detailed analysis using e.g. techniques of [5] or [9] is necessary.

6. Implementation
All the above experiments have been performed with the Munich Multigrid Workbench (see [7]). The workbench is a prototype software package for the programming of multigrid methods. Its main features are:

- Convenience: With the workbench a standard multigrid algorithm can be formulated in less than twenty lines of code.
- Safety: The formulation of the algorithms is in terms of gridfunctions and operators. There is no possibility to make low level errors with e.g. arrays and indices.
- Convenient debug facilities: Each step of the algorithm can be performed separately and analyzed separately. Intermediate results can be displayed graphically, algorithms can be traced, etc.
- Portability: The package is fully portable within the UNIX environment.
- Flexibility: The approach is not restricted to any class of problems. It has been used for variable coefficient convection diffusion problems in two dimensions and is presently being extended to include three dimensional problems.
- Efficiency: The workbench has been used to solve large problems with $10^8$ unknowns on microcomputers.
- Parallelism: The workbench is designed to make use of multiprocessor architectures and may be used for distributed computations.

7. Acknowledgements
The author wishes to thank Prof. Dr. Zenger for many stimulating discussions and P. Muszyński for several helpful comments.

References
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