Extrapolation Techniques for Computing Accurate Solutions of Elliptic Problems with Singular Solutions

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Abstract. Generalized functions occur in many practical applications as source terms in partial differential equations. Typical examples are point loads and dipoles as source terms for electrostatic potentials. For analyzing the accuracy of such computations, standard techniques cannot be used, since they rely on global smoothness. At the singularity, the solution tends to infinity and therefore standard error norms will not even converge.

In this article we will demonstrate that these difficulties can be overcome by using other metrics to measure accuracy and convergence of the numerical solution. Only minor modifications to the discretization and solver are necessary to obtain the same asymptotic accuracy and efficiency as for regular and smooth solutions. In particular, no adaptive refinement is necessary and it is also unnecessary to use techniques which make use of the analytic knowledge of the singularity. Our method relies simply on a mesh-size dependent representation of the singular sources constructed by appropriate smoothing. It can be proved that the pointwise accuracy is of the same order as in the regular case. The error coefficient depends on the location and will deteriorate when approaching the singularity where the error estimate breaks down. Our approach is therefore useful for accurately computing the global solution, except in a small neighborhood of the singular points. It is also possible to integrate these techniques into a multigrid solver exploiting additional techniques for improving the accuracy, such as Richardson and τ-Extrapolation.

1 Introduction

Typical error estimates for the numerical solution of boundary value problems depend on the smoothness of the true solution which is not given in many practical applications. Reasons for such singular solutions can for example be reentrant corners, discontinuous coefficients, singular functions in the boundary conditions or source terms with singularities. In this article we consider the last case. As application we choose for simplicity electrostatic potentials of point loads, physically modeled by the Maxwell equations in the vacuum (cf. [1]). The method

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is extensible to more general situations, but the basic idea of the method is presented here in terms of this simple example. It leads to the **Poisson equation** with Dirichlet boundary conditions in the unit cube $\Omega = [0,1]^3 \subset \mathbb{R}^3$

$$\begin{aligned} -\Delta u &= f \text{ in } \Omega \\ u &= g \text{ on } \partial\Omega \end{aligned} , \tag{1}$$

where Δ is the Laplace operator, $\partial\Omega$ denotes the boundary of Ω and g is a smooth function. The source term f contains one or more singularities, because a point load is modeled by the Dirac δ-function. As an extension we will consider sources containing dipoles and quadrupoles. A dipole can formally introduced as a directional derivative of a point load, a quadrupole as a directional derivative of a dipole. So we have to study the Dirac δ-function and its derivatives in order to solve problem (1). Note that the Dirac δ-function is not a function in the common sense (cf. [2]). To be able to deal with it the concept of a function is extended to the concept of a distribution or generalized function (cf. [3]).

For the discretization of (1) we use finite differences on equidistant grids with mesh size $h = \frac{1}{N}$. The discrete Laplace operator is given by the usual 7-point stencil (cf. [4], p.71).

The question now is how to discretize the right hand side f containing the singularity. f is equal to zero on every point in Ω except at the singularity where it is ∞. If we assume that the singularity is not located at a grid point, simply set $f_h \equiv 0$ and then try to solve the above problem without any modifications and a standard solver, we would get poor results. On the one hand, standard error norms near the singularity will not converge, because the solution at the singularity is unbounded, and on the other hand the accuracy is destroyed in the whole domain by the singularity. This phenomenon is called **pollution effect**.

In section 2 we present the **Zenger Correction Method** to overcome the pollution effect. The idea is to represent the singular generalized components of f by grid-adapted B-Splines. Extending results from [5] we can show that the pollution effect can be eliminated leading to errors of the same quality and convergence rate as for smooth problems. Its great advantage is that we do not need to know the exact singular component of the solution of the problem to approximate the singularity. Therefore it can be used for a variety of problems.

In section 3 the core theorems for the error estimates of the discretization error for the Poisson equation in the unit cube are presented and the proof of the main result is outlined.

In section 4 we further improve the accuracy of the numerical solution by using extrapolation. Two extrapolation methods, namely Richardson extrapolation and τ-extrapolation are briefly described in combination with the Zenger Correction.

In the 5th section the experimental results for the numerical solution of the Poisson equation with Zenger Correction are summarized.

2 Singular Source Terms in Poisson's Equation

The Zenger Correction Method uses the following generalized functions (cf. [2]) in order to approximate the physical singularities contained in the right hand side f of equation (1).

Definition 1 (Generalized functions H_i). *Let $H_0 : \mathbb{R} \to \mathbb{R}$ be the* ***Heaviside-function***

$$H_0(x) := \begin{cases} 0 & : \quad x \leq 0 \\ 1 & : \quad x > 0 \end{cases} , \tag{2}$$

and the distributions H_i, $i \in \mathbb{Z}$, be recursively defined by

$$H_i(x) := \begin{cases} \frac{d}{dx} H_{i-1}(x) & : \quad i > 0 \\ \int_{-\infty}^{x} H_{i+1}(\xi) d\xi & : \quad i < 0 \end{cases} . \tag{3}$$

The family of functions H_i enables us to represent arbitrary physical multipoles. For example H_1 corresponds to the Dirac δ-function, resp. a point load. Remember that the directional derivative of a point load was defined as a special dipole. For higher dimensions we use tensor products of these functions. For the two multi indices $\boldsymbol{x}_0 = (x_{0,1}, x_{0,2}, \ldots , x_{0,n}) \in \mathbb{R}^n$ that indicates the location of the singularity and $\boldsymbol{a} = (a_1, a_2, \ldots , a_n) \in \mathbb{Z}^n$ that specifies the functions H_i we use the notation

$$\mathcal{H}_{\boldsymbol{x}_0}^{\boldsymbol{a}}(\boldsymbol{x}) = \prod_{i=1}^{n} H_{a_i}(x_i - x_{0,i}) . \tag{4}$$

The idea of the Zenger Correction Method is now to **integrate** the right hand side f **analytically** a number of times, until the result is a product of smooth functions H_i with $i < 0$. Then we **differentiate** this function **numerically** as often as we had integrated it. This results in a approximation to the singularity which becomes more accurate with smaller mesh size h. For the numerical differentiation we use finite differences with the notation

$$\delta^{\boldsymbol{i}} = \delta_{x_1}^{i_1} \circ \delta_{x_2}^{i_2} \circ \cdots \circ \delta_{x_n}^{i_n} , \tag{5}$$

for the multi index $\boldsymbol{i} \in \mathbb{Z}^n$ that indicates how often we differentiate in each direction. Dependent on the number of integrations resp. differentiation steps n we call that procedure the **Zenger Correction of n-th order**. In general for even n with $k - n < 0$ we have

$$\delta_x^n H_k(x) = \begin{cases} 0 & : \quad |x| \geq \frac{n}{2} h \\ \frac{1}{h^n} \sum_{i=0}^{n} (-1)^i \binom{n}{i} H_{k-n}(x + (i - \frac{n}{2})h) & : \quad |x| < \frac{n}{2} h \end{cases} . \tag{6}$$

One can show that (6) is identical to a B-Spline (cf. [6]).

3 Error Estimates

In this section we prove that if the singularity in the source term is replaced by the above approximation, we obtain an $O(h^2)$ discretization error as in the smooth case, except in a small area near the singularity.

Definition 2 (H-bounded). *A family of functions $u_h(\boldsymbol{x})$ is called* ***h-bounded*** *on the domain $\Omega \subset \mathbb{R}^n$, if there exists a real valued, continuous function $r(\boldsymbol{x})$ on Ω which is not necessarily bounded on Ω, so that for every $\boldsymbol{x} \in \Omega$ there exists a number $h_0 > 0$ with $|u_h(\boldsymbol{x})| \leq r(\boldsymbol{x})$ for all $h = \frac{1}{N} < h_0, N \in \mathbb{N}$, $\boldsymbol{x} \in \Omega_h$. If $r(\boldsymbol{x})$ is bounded on Ω, $u_h(\boldsymbol{x})$ is called* ***strictly h-bounded*** *(cf. [7], p.6).*

A h-bounded family of grid functions u_h may be unbounded on Ω for $h \to 0$, but because of the continuity of r be bounded for all $h > 0$ on every compact subset of Ω.

Theorem 1. *Let the solution of $\Delta_h u_h = f_h$ in Ω_h be bounded on $\overline{\Omega}_h$. If $\delta^{2\boldsymbol{i}} f_h$ is h-bounded on Ω and for all i_l, m_l with $0 \leq i_l \leq m_l$ for $0 < l \leq n$, then $\delta^{2\boldsymbol{m}} u_h$ is h-bounded on Ω.*

The proof of this theorem is found in [8] for the 2D case and will be generalized to 3D in a forthcoming paper.

Now we are prepared for the central theorem.

Theorem 2. *Let u^* be the (weak) solution of the boundary value problem*

$$\begin{aligned} \Delta u &= \mathcal{H}^{\boldsymbol{a}}_{\boldsymbol{x}_0}(\boldsymbol{x}) \text{ in } \Omega \\ u &= 0 \qquad\quad \text{on } \partial\Omega \end{aligned} , \tag{7}$$

where $\mathcal{H}^{\boldsymbol{a}}_{\boldsymbol{x}_0}(\boldsymbol{x})$ is a singularity located in $\boldsymbol{x}_0 \in \Omega = [0,1]^n$. $n \in \{2,3\}$ is the dimension of the problem. Let u_h^* the solution of

$$\begin{aligned} \Delta_h u_h &= f_h \text{ in } \Omega_h \\ u_h &= 0 \quad \text{on } \partial\Omega_h \end{aligned} , \tag{8}$$

where $f_h = \delta^{2\boldsymbol{m}} \mathcal{H}^{\boldsymbol{a}-2\boldsymbol{m}}_{\boldsymbol{x}_0}(\boldsymbol{x})$, and where $\boldsymbol{m}$ is chosen componentwise such that $2m_l > a_l$ for $1 \leq l \leq n$. By definition it follows that $\mathcal{H}^{\boldsymbol{a}-2\boldsymbol{m}}_{\boldsymbol{x}}$ are continuous functions. Then:

$$u_h^* = u^* + h^2 r$$

where r is h-bounded on $\Omega \backslash \{\boldsymbol{x}_0\}$.

The proof can be found in [5], pp.15 and can be extended to the 3D case.

The advantages of the Zenger Correction Method are that no modification of the grid or the solver is necessary. Furthermore the number of points that have to be corrected is fixed and does not depend on the mesh size h. The analytic solution is not needed to construct the correction.

Note that the Zenger Correction Method eliminates the pollution effect. This results in a (pointwise) $\mathcal{O}(h^2)$ accuracy at any fixed distance from the singular point. However, the method cannot provide locally good accuracy. This is impossible since the true solution tends to infinity where the singularity is located.

4 Extrapolation

In this section we present two extrapolation methods in order to improve the discretization error from $\mathcal{O}(h^2)$ to $\mathcal{O}(h^4)$.

4.1 Richardson Extrapolation

Richardson Extrapolation can be used if there exist asymptotic expansions of the discretization error (cf. [9]). In this case the solutions of different mesh sizes can be combined to eliminate the lower order terms. For our problem we use the mesh sizes h und $H = 2h$. In order to get the higher accuracy on the coarse grid we change the values there by

$$\widehat{\boldsymbol{u}}_H^* = \frac{4}{3}\mathcal{I}_h^H \boldsymbol{u}_h^* - \frac{1}{3}\boldsymbol{u}_H^* \ , \tag{9}$$

where $\mathcal{I}_h^H$ is an injection operator. The existence of such asymptotic expansions can be proved even in the case of singularities by extension of Theorem 2.

4.2 τ-Extrapolation

τ-Extrapolation is a multigrid specific technique that in contrast to Richardson extrapolation works only on a single grid. It is based on the principle of **defect correction** and has been first mentioned by Brandt (cf. [10], see also Hackbusch [11], pp.278).

In the CS(correction scheme)-Multigrid algorithm two different iterations are used alternately, the smoother and the coarse grid correction (cf. [4]). These two iterations have a common fixed point described by $\boldsymbol{f}_h - \boldsymbol{A}_h \boldsymbol{u}_h = 0$ (cf. [5], p. 17f). The smoother converges fast for certain (usually the high frequency) solution components, but converges only slowly for the remaining (low frequency) modes. The coarse grid correction behaves vice versa. If these complementary properties are combined the typical multigrid efficiency is obtained.

Now we follow the idea of **double discretization**, i.e. in the coarse grid correction process higher order discretizations are used. Using a correction of the form

$$\boldsymbol{u}_h^{(k+1)} = \boldsymbol{u}_h^{(k)} + \boldsymbol{e}_h^{(k)} \ , \tag{10}$$

where $\boldsymbol{e}_h^{(k)}$ is computed as a coarse grid correction

$$\boldsymbol{e}_h^{(k)} = \mathcal{I}_H^h \boldsymbol{A}_H^{-1} \widehat{\mathcal{I}}_h^H (\boldsymbol{f}_h - \boldsymbol{A}_h \boldsymbol{u}_h^{(k)}) \ , \tag{11}$$

would lead to a standard multigrid method. τ-extrapolation consists in using a linear combination of fine and coarse grid residual to construct an extrapolated correction

$$\widehat{\boldsymbol{u}}_h^{(k+1)} = \boldsymbol{u}_h^{(k)} + \mathcal{I}_H^h \boldsymbol{A}_H^{-1}\left(\frac{4}{3}\widehat{\mathcal{I}}_h^H(\boldsymbol{f}_h - \boldsymbol{A}_h \boldsymbol{u}_h^{(k)}) - \frac{1}{3}(\widehat{\mathcal{I}}_h^H \boldsymbol{f}_h - \boldsymbol{A}_H \mathcal{I}_h^H \boldsymbol{u}_h^{(k)})\right) \ . \quad (12)$$

It can be shown that this modification of the coarse grid correction leads to a numerical error of order $\mathcal{O}(h^4)$ (cf. [12]). The modified coarse grid correction is only applied on the finest grid once per V-cycle. Additionally we have to take care when choosing the restriction and the interpolation operators. Normally trilinear interpolation for $\mathcal{I}_H^h$, full weighting for $\widehat{\mathcal{I}}_h^H$ and injection for $\mathcal{I}_h^H$ is used, but this can vary from problem to problem. One has also to pay attention not do do too many post smoothing steps, because this can destroy the higher accuracy. For the Poisson equation with singular source term we have to discretize the right hand side on each grid due to the fact that the restriction of the B-spline cannot approximate the right hand side well enough on the coarse grid. A concise analysis of the τ-extrapolation is e.g. found in [12].

5 Experimental Results for a Point Load in 3D

For the experiments we use CS-Multigrid as solver, e.g $CS(2,2,15)$ means that we do 2 presmoothing and 2 postsmoothing steps and a maximum of 15 V-cycles (cf. [13]). The singularity is located at $\boldsymbol{x}_0 = (0.26, 0.26, 0.26)^T$ in the domain $\Omega = [0,1]^3$. To evaluate the accuracy away from the singularity we will consider $\Omega \setminus R$, where $R = [0.125, 0.375]^3$ is a fixed neighbourhood of $\boldsymbol{x}_0$.

The analytical solution of the Poisson equation in 3D with a point load as source term is given by

$$u_p^*(\boldsymbol{x}) = -\frac{1}{4\pi|\boldsymbol{x}|} \ . \quad (13)$$

The boundary value problem with Zenger Correction of 4th order is described by

$$\begin{aligned} -\Delta u(\boldsymbol{x}) &= \mathcal{H}_{\boldsymbol{x}_0}^{(1,1,1)}(\boldsymbol{x}) \quad \text{in } \Omega \\ u(\boldsymbol{x}) &= u_p^*(\boldsymbol{x}) + g(\boldsymbol{x}) \text{ on } \partial\Omega \end{aligned} \quad (14)$$

with its discretization

$$\begin{aligned} -\Delta_h u_h(\boldsymbol{x}) &= \delta^{(4,4,4)}\mathcal{H}_{\boldsymbol{x}_0}^{(-3,-3,-3)}(\boldsymbol{x}) \text{ in } \Omega_h \\ u_h(\boldsymbol{x}) &= u_{p,h}^*(\boldsymbol{x}) + g_h(\boldsymbol{x}) \qquad \text{on } \partial\Omega_h \end{aligned} \ , \quad (15)$$

where $g(\boldsymbol{x}) = \sin(x\pi)\sin(y\pi)\sinh(\sqrt{2}z\pi)$. Table 1 lists the numerical results. The first column shows the mesh size h, the second the maximum norm of the discretization error, then follow the L_1 resp. L_2 norms in the whole domain Ω and in the domain $\Omega \setminus R$. The small numbers between the rows of the table show the numerical convergence rates α which are for a point $\boldsymbol{p} \in \Omega$ computed by

$$\alpha = (\ln|u^*(\boldsymbol{p}) - u_h(\boldsymbol{p})| - \ln|u^*(\boldsymbol{p}) - u_{h/2}(\boldsymbol{p})|)/(\ln 2) \quad (16)$$

and analogous for the norms in the other columns.

Table 1. Convergence rates of the discretization error.

h	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	rate	L_∞	L_1 Ω	rate	L_2 Ω	rate	L_1 $\Omega\backslash R$	rate	L_2 $\Omega\backslash R$	rate
$\frac{1}{16}$	4.81e-02	2.0	2.67e+00	2.04e-02	2.1	5.28e-02	2.4	1.98e-02	2.1	2.61e-02	2.1
$\frac{1}{32}$	1.21e-02	2.0	1.22e+00	4.61e-03	2.0	9.89e-03	1.2	4.52e-03	2.1	6.22e-03	2.0
$\frac{1}{64}$	3.02e-03	2.0	1.69e+00	1.12e-03	2.0	4.34e-03	-0.2	1.08e-03	2.0	1.52e-03	2.0
$\frac{1}{128}$	7.55e-04	2.0	6.92e+00	2.78e-04	2.0	5.07e-03	1.9	2.63e-04	2.0	3.74e-04	2.0
$\frac{1}{256}$	1.89e-04		3.21e+00	6.91e-05		1.39e-03		6.50e-05		9.30e-05	

Using an additional Richardson extrapolation or additional τ-extrapolation for solving problem (14) we obtain the improved accuracy rates, as shown in Table 2 and 3, respectively.

Table 2. Convergence rates of the discretization error with Richardson extrapolation.

h	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	rate	L_∞	L_1 Ω	rate	L_2 Ω	rate	L_1 $\Omega\backslash R$	rate	L_2 $\Omega\backslash R$	rate
$\frac{1}{16}$	5.77e-05	4.0	7.30e-01	3.89e-04	3.6	1.28e-02	2.9	3.44e-05	3.9	5.32e-05	3.5
$\frac{1}{32}$	3.70e-06	4.0	2.55e-01	3.19e-05	2.4	1.69e-03	1.0	2.28e-06	3.9	4.66e-06	3.7
$\frac{1}{64}$	2.33e-07	4.0	3.79e-01	6.14e-06	1.6	8.71e-04	-0.0	1.48e-07	4.0	3.56e-07	3.9
$\frac{1}{128}$	1.44e-08		1.03e+00	1.97e-06		8.77e-04		9.21e-09		2.36e-08	

Table 3. Convergence rates of the discretization error with τ-extrapolation.

h	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	rate	L_∞	L_1 Ω	rate	L_2 Ω	rate	L_1 $\Omega\backslash R$	rate	L_2 $\Omega\backslash R$	rate
$\frac{1}{16}$	1.67e-03	3.9	2.64e+00	2.54e-03	3.4	4.57e-02	2.6	1.54e-03	3.9	2.61e-03	3.8
$\frac{1}{32}$	1.12e-04	4.0	1.18e+00	2.46e-04	2.5	7.43e-03	0.9	1.01e-04	4.0	1.85e-04	3.9
$\frac{1}{64}$	7.24e-06	4.0	1.66e+00	4.30e-05	2.0	3.94e-03	-0.3	6.46e-06	4.0	1.23e-05	3.9
$\frac{1}{128}$	4.58e-07	4.0	6.85e+00	1.10e-05	2.3	4.97e-03	1.9	4.09e-07	4.0	8.00e-07	4.0
$\frac{1}{256}$	2.86e-08		3.09e+00	2.17e-06		1.30e-03		2.55e-08		5.02e-08	

6 Conclusion

In this paper we have presented the basic idea of the Zenger Correction Method including some simple examples. More examples, i.e. problems with dipoles and quadrupoles can be found in [6]. Furthermore a concise mathematical analysis of the Zenger Correction will be presented in a forthcoming paper.

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