The Theory of Difference Potentials in the Three-Dimensional Case

Angela Hommel

In the following a discrete method to solve elliptic boundary value problems will be presented. In analogy to the classical potential theory, the main idea consists in solving an equation on the boundary, where the equivalence to the original problem is preserved. In the classical case this boundary equation is an integral equation, which can not immediately be solved. In general a quadrature formula is used to calculate an approximate solution of the integral equation. In the discrete case, where all derivatives are approximated by finite differences, the boundary equation is a linear equation system. This equation system can be solved exactly. Using the discrete single-layer or double-layer potential the solution can be calculated at the mesh points of the interior or exterior domain. The described method of difference potentials is based on the discrete Laplace equation in the three-dimensional case. In order to give only a survey of this theory the main results are presented without any proof.

1. Introduction

Let R^3 be the three-dimensional Euclidean space. An equidistant lattice of the mesh width $h > 0$ is defined by $\mathrm{R}_h^3 = \{mh = (m_1 h, m_2 h, m_3 h):\ m_i \in Z\ ,\ i = 1,2,3\}$. In the following the domain $G \in \mathrm{R}^3$ is bounded and simply connected with a piecewise smooth boundary Γ. To describe the method of difference potentials the set $M = \left\{ m = (m_1, m_2, m_3):\ m_i \in Z,\ i = 1,2,3,\ (m_1 h, m_2 h, m_3 h) \in \left(G \cap \mathrm{R}_h^3\right) \right\}$ and the set $K = \{(0,0,0), (-1,0,0), (1,0,0), (0,-1,0), (0,1,0), (0,0,-1), (0,0,1)\}$ are introduced. For all points $m \in M$ the seven-point star $N_m = \{m + k:\ k \in K\}$ is considered. The union $\bigcup_{m \in M} N_m$ is denoted by N. Furthermore at all points $r = (r_1, r_2, r_3) \in N$ the set $K_r = \{k \in K:\ r + k \notin M\}$ is defined. Similar to the bounded domain G the discrete domain $G_h = \{(m_1 h, m_2 h, m_3 h):\ m = (m_1, m_2, m_3) \in M\}$ with the double-layer boundary $\gamma_h = \{rh:\ r \in N \text{ and } K_r \neq \emptyset\}$ will be studied. In more detail the mesh points rh, in which the set K_r contains the element $k = (0,0,0)$, are mesh points of the outer boundary layer γ_h^-. The mesh points $rh \in \gamma_h \setminus \gamma_h^-$ are points of the inner boundary layer γ_h^+. There is to remark, that the outer edges of the domain do not play any role in this theory.

In the following the difference equation

$$-\Delta_h u_h(mh) = \sum_{k \in K} a_k u_h(mh - kh) = f_h(mh) \qquad \forall mh \in G_h$$

with

$$a_k = \begin{cases} -1/h^2 & \text{for } k \in K,\ k \neq (0,0,0) \\ 6/h^2 & \text{for } k = (0,0,0) \end{cases}$$

is considered.

The basis to develop a discrete potential theory is the existence of the discrete fundamental solution $E_h(mh)$, which fulfils the equation

$$-\Delta_h E_h(mh) = \begin{cases} 1/h^3 & \text{if } \ mh = (0,0,0) \\ 0 & \text{if } \ mh \neq (0,0,0). \end{cases}$$

This discrete fundamental solution can be calculated by the help of the discrete Fourier transform. The obtained integral representation has the form

$$E_h(mh) = \frac{1}{(2\pi)^3} \int_{Q_h} \frac{e^{-imh\xi}}{d^2} \, d\xi \qquad \text{with}$$

$$d^2 = \frac{4}{h^2}\left(\sin^2 \frac{h\xi_1}{2} + \sin^2 \frac{h\xi_2}{2} + \sin^2 \frac{h\xi_3}{2}\right) \text{ and } Q_h = \left\{\xi \in \mathrm{R}^3 : -\frac{\pi}{h} < \xi_i < \frac{\pi}{h},\ i = 1,2,3\right\}.$$

Additionally at each mesh point $mh \in \mathrm{R}_h^3$ the inequality $|E_h(mh)| \leq \frac{C}{|mh| + h}$ can be proved (see [4]). In relation with the continuous fundamental solution

$$E(x) = \frac{1}{(2\pi)^3} \int_{\mathrm{R}^3} \frac{e^{-ix\xi}}{|\xi|^2} \, d\xi = \frac{1}{4\pi |x|}$$

an estimation in the form $|E_h(mh) - E(mh)| \leq \frac{C\,h}{|mh|^2}$ is possible $\forall m \neq (0,0,0)$. Furthermore for each mesh width $h \leq e^{-1}$ it can be proved that

$$\| E_h(mh) - E(mh) \|_{l_p(G_h^*)} = \left(\sum_{mh \in G_h^*} |E_h(mh) - E(mh)|^p \, h^3 \right)^{\frac{1}{p}} \leq \begin{cases} C(L)\,h & 1 \leq p < 3/2 \\ C\,h |\ln h|^{2/3} & p = 3/2 \\ C\,h^{-1+3/p} & 3/2 < p < 3, \end{cases}$$

where $G_h^* = \{mh \in G_h : mh \neq (0,0,0)\}$ and $L = 2lh$ is the length of the smallest cube $Q(G_h)$ with the center $(0,0,0)$, which covers the discrete domain G_h. By the same way it follows

$$\| E_h(mh) - E(mh) \|_{l_p(\mathrm{R}_h^3 \setminus (0,0,0))} \leq C\, h^{-1+3/p} \quad \text{for} \quad 3/2 < p < 3.$$

If the discrete fundamental solution is not only considered at the mesh points $mh \in \mathrm{R}_h^3$, then the convergence of the discrete fundamental solution can be investigated in the space L_p, too. In more detail for $2 \leq p < 3$ it can be proved that

$$\begin{aligned} &E_h(x) \to E(x) && \text{in } L_p(G) && \text{for } h \to 0 \quad \text{and} \\ &E_h(x) - E(x) \to 0 && \text{in } L_p(\mathrm{R}^3) && \text{for } h \to 0. \end{aligned}$$

2. Difference Potentials

The numerical algorithm for solving elliptic boundary value problems is based on the following ideas. The discrete analogue of the integral representation for functions in C^2 can be written in the form

$$\sum_{rh\in\gamma_h}\left(\sum_{k\in K_r} E_h(lh-(r+k)h)\,a_k\,h^3\right)u_h(rh)-\sum_{m\in M} E_h(lh-mh)\,\Delta_h u_h(mh)\,h^3=\begin{cases}u_h(lh) & l\in N\\ 0 & l\notin N.\end{cases}$$

If the boundary values on γ_h^- are denoted by $u_R(rh)=u_h(rh)$ and the discrete normal derivatives are defined by $u_A(rh)=h^{-1}\sum_{k\in K\setminus K_r}\left(u_h(rh)-u_h((r+k)h)\right)$, then it can be proved that

$$\sum_{rh\in\gamma_h}\left(\sum_{k\in K_r} E_h(lh-(r+k)h)\,a_k\,h^3\right)u_h(rh)=\left(P_h^E\,u_A\right)(lh)-\left(P_h^D\,u_R\right)(lh)$$

with the discrete single-layer potential $\left(P_h^E\,u_A\right)(lh)=\sum_{rh\in\gamma_h^-}u_A(rh)E_h(lh-rh)h^2$ and the discrete double-layer potential

$$\left(P_h^D\,u_R\right)(lh)=\sum_{rh\in\gamma_h^-}\sum_{k\in K\setminus K_r}\frac{E_h(lh-rh)-E_h(lh-(r+k)h)}{h}u_R(rh)h^2-\chi\,u_R(lh).$$

There is $\chi=0,$ if $lh\in G_h$ and $\chi=1,$ if $lh\in\gamma_h^-$.
This difference potentials are the basis to find a special ansatz for the equation system on the boundary and to calculate the solution of the boundary value problem at the mesh points inside the domain.

The potential $\left(P_h^E\,u_A\right)(lh)$ as well as the potential $\left(P_h^D\,u_R\right)(lh)$ are *discrete harmonic functions in the domain* G_h, that means functions with the properties $-\Delta_h\left(P_h^E\,u_A\right)(lh)=0$ or $-\Delta_h\left(P_h^D\,u_R\right)(lh)=0 \quad \forall lh\in G_h$, respectively.

To prove uniqueness theorems, the discrete analogues of the first and second Green's formula will be considered.

Because the potential theory can be used to solve exterior boundary value problems in a very simply way, the main ideas in the discrete case will be presented now.

Let $G^a\in\mathrm{R}^3$ be a bounded exterior domain with a piecewise smooth boundary. In analogy to the symbols in section 1, the discrete domain G_h^a with the double-layer boundary $\gamma_h^a=\gamma_h^{a-}\cup\gamma_h^{a+}$ is considered. To describe this domain, the sets $M^a=\left\{m=(m_1,m_2,m_3): m_i\in Z,\, i=1,2,3,\; mh\in\left(G^a\cap R_h^3\right)\right\}$, $K_r^a=\left\{k\in K: r+k\notin M^a\right\}$,

$N_m = \{ m + k : k \in K \}$, $N^a = \bigcup_{m \in M^a} N_m$ and the set $\gamma_h^a = \{ rh : r \in N^a \text{ with } K_r^a \neq \emptyset \}$ of the mesh points on the boundary are introduced. If the boundary values on γ_h^{a-} are denoted by $u_R(rh) = u_h(rh)$ and the discrete normal derivatives are defined by $u_A(rh) = h^{-1} \sum_{k \in K \setminus K_r^a} (u_h(rh) - u_h((r+k)h))$, then the discrete single-layer potential can be written in the form $(P_h^{E,a} u_A)(lh) = \sum_{rh \in \gamma_h^{a-}} u_A(rh) E_h(lh - rh) h^2$, while the discrete double-layer potential has the representation

$$(P_h^{D,a} u_R)(lh) = \sum_{rh \in \gamma_h^{a-}} \sum_{k \in K \setminus K_r^a} \frac{E_h(lh - rh) - E_h(lh - (r+k)h)}{h} u_R(rh) h^2 - \chi u_R(lh)$$

with $\chi = 0$, if $lh \in G_h^a$ and $\chi = 1$, if $lh \in \gamma_h^{a-}$. There is to remark, that in general $\gamma_h^{a-} \neq \gamma_h^-$ is valid. By the help of this potentials it can be proved that

$$(P_h^{E,a} u_A)(lh) - (P_h^{D,a} u_R)(lh) - \sum_{m \in M^a} E_h(lh - mh) \Delta_h u_h(mh) h^3 = \begin{cases} u_h(lh) & l \in N^a \\ 0 & l \notin N^a . \end{cases}$$

In the three-dimensional case a function $u_h(mh)$ is called *discrete harmonic in an exterior domain*, if at each mesh point $mh \in G_h^a$ the equation $-\Delta_h u_h(mh) = 0$ is fulfilled and additionally the inequality $|u_h(mh)| \leq C |mh|^{-1}$ as $|mh| \to \infty$ is valid with an arbitrary constant $C < \infty$. The discrete single- and double-layer potential are discrete harmonic functions in the exterior domain.

3. Uniqueness Theorems

In this section the four kinds of discrete boundary value problems are presented, which will be solved in the following.

Interior Dirichlet Problem (D_i)**:** The boundary value problem

$$\begin{aligned} -\Delta_h u_h(mh) &= 0 & \forall mh \in G_h \\ u_h(rh) &= \varphi_h(rh) & \forall rh \in \gamma_h^- \end{aligned}$$

has a unique solution for arbitrary boundary values $\varphi_h(rh)$.

Interior Neumann Problem (N_i)**:** The solution of the problem

$$\begin{aligned} -\Delta_h u_h(mh) &= 0 & \forall mh \in G_h \\ h^{-1} \sum_{k \in K \setminus K_r} (\mathrm{u_h}(rh) - u_h((r+k)h)) &= \psi_h(rh) & \forall rh \in \gamma_h^- \end{aligned}$$

is unique up to a constant, if the necessary condition $\sum_{rh \in \gamma_h^-} \psi_h(rh) h^2 = 0$ is fulfilled.

Exterior Dirichlet Problem (D_a)**:** The discrete problem

$$\begin{aligned} -\Delta_h u_h(mh) &= 0 && \forall mh \in G_h^a \\ |u_h(mh)| &\leq C|mh|^{-1} && \text{for } |mh| \to \infty \\ u_h(rh) &= \varphi_h^a(rh) && \forall rh \in \gamma_h^{a-} \end{aligned}$$

can be uniquely solved for arbitrary boundary values $\varphi_h^a(rh)$.

Exterior Neumann Problem (N_a)**:** If the necessary condition $\sum_{rh \in \gamma_h^{a-}} \psi_h^a(rh) h^2 = 0$ is fulfilled, then the solution of the boundary value problem

$$\begin{aligned} -\Delta_h u_h(mh) &= 0 && \forall mh \in G_h^a \\ |u_h(mh)| &\leq C|mh|^{-1} && \text{for } |mh| \to \infty \\ h^{-1} \sum_{k \in K \setminus K_r^a} \left(u_h(rh) - u_h((r+k)h)\right) &= \psi_h^a(rh) && \forall rh \in \gamma_h^{a-} \end{aligned}$$

is unique up to a constant.

4. The Equation Systems on the Boundary

In the following the linear equation systems on the boundary are presented, which are equivalent to the discrete boundary value problems. These formulas are based on the discrete single-layer potential.

4.1. Interior Dirichlet Problem

Theorem 1: If it is possible to solve the linear equation system

$$\varphi_h(lh) = \sum_{rh \in \gamma_h^-} v_h(rh) E_h(lh - rh) h^2 \qquad \forall lh \in \gamma_h^- ,$$

then the single-layer potential $(P_h^E v_h)(mh) = \sum_{rh \in \gamma_h^-} v_h(rh) E_h(mh - rh) h^2$ is a solution of the interior Dirichlet problem at each mesh point $mh \in (G_h \cup \gamma_h^-)$.

Theorem 2: The linear equation system in Theorem 1 has a unique solution for arbitrary boundary values $\varphi_h(lh)$ on γ_h^-.

4.2. Interior Neumann Problem

Theorem 3: If the equation system

$$\psi_h(lh) = \sum_{k \in K \setminus K_l} \sum_{rh \in \gamma_h^-} \left(E_h(lh - rh) - E_h((l+k)h - rh)\right) v_h(rh) h \qquad \forall lh \in \gamma_h^- ,$$

can be solved and the necessary condition is fulfilled, then $\forall mh \in \left(G_h \cup \gamma_h^-\right)$ the potential $\left(P_h^E v_h\right)(mh) = \sum_{rh \in \gamma_h^-} v_h(rh) E_h(mh - rh) h^2$ is a solution of the problem $\left(N_i\right)$.

Theorem 4: The condition $\sum_{rh \in \gamma_h^-} \psi_h(rh) h^2 = 0$ is necessary and sufficient for the solvability of the equation system in theorem 3.

4.3. Exterior Dirichlet Problem

Theorem 5: If the solution of the system $\varphi_h^a(lh) = \sum_{rh \in \gamma_h^{a-}} v_h(rh) E_h(lh - rh) h^2$ exists $\forall lh \in \gamma_h^{a-}$, then the single-layer potential $\left(P_h^{E,a} v_h\right)(mh) = \sum_{rh \in \gamma_h^{a-}} v_h(rh) E_h(mh - rh) h^2$ is a solution of the exterior Dirichlet problem at each mesh point $mh \in \left(G_h^a \cup \gamma_h^{a-}\right)$.

Theorem 6: For arbitrary chosen boundary values $\varphi_h^a(lh)$ on γ_h^{a-} the equation system in Theorem 5 has a unique solution.

4.4. Exterior Neumann Problem

Theorem 7: If the necessary condition is fulfilled and the equation system

$$\psi_h^a(lh) = \sum_{k \in K \setminus K_l^a} \sum_{rh \in \gamma_h^{a-}} \left(E_h(lh - rh) - E_h((l + k)h - rh)\right) v_h(rh) h \qquad \forall lh \in \gamma_h^{a-},$$

can be solved, then the single-layer potential $\left(P_h^{E,a} v_h\right)(mh) = \sum_{rh \in \gamma_h^{a-}} v_h(rh) E_h(mh - rh) h^2$ is a solution of the exterior Neumann problem at each mesh point $mh \in \left(G_h^a \cup \gamma_h^{a-}\right)$.

Theorem 8: For arbitrary discrete normal derivatives $\psi_h^a(lh)$ on γ_h^{a-} with $\sum_{rh \in \gamma_h^{a-}} \psi_h^a(rh) h^2 = 0$ the linear equation system in Theorem 7 has a unique solution.

5. References

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