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Difference Potentials and Their Applications

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DIFFERENCE POTENTIALS AND THEIR APPLICATIONS*

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Abstract. In this lecture, we introduce the concept of difference potentials with the density from the space of discontinuities or jumps, which extends and generalizes the previous constructions of difference potentials; this new concept is sufficiently universal and at the same time simple. The apparatus of difference potentials constitutes the foundation of the difference potentials method (DPM).

Before considering the actual constructions of difference potentials, we discuss some new opportunities that the DPM provides for computations. This brief introductory discussion (as well as the main part of the lecture itself) has a goal of drawing the attention of the scientific computing research community to the DPM and its applications. Although the construction of difference potentials with the density from the space of jumps presents an independent mathematical interest, the subject of this lecture will seem too abstract without discussing the possible applications in the beginning. Moreover, in the end of the lecture we will give a review of the literature emphasizing some applications of the DPM that have already been implemented in computational practice.

Key words. difference potentials method, boundary-value problems, domain decomposition, active sound control

Subject classification. Applied and Numerical Mathematics

1. Introduction. The DPM extends the capabilities of both the classical finite difference method (FDM) and the boundary elements method (BEM). Let us first compare the DPM against FDM. It is well known that the problems most suited for the solution by the FDM are those formulated on the geometrically simple, e.g., rectangular, domains and discretized on the simple structured, e.g., Cartesian, grids. In this case, the resulting finite-difference schemes typically appear easily parallelizable as well. The DPM allows one to use these simplest finite-difference schemes for the numerical solution of linear PDE's/systems on the domains with curvilinear boundary and for the case of general boundary conditions. Moreover, it should be emphasized that the DPM does not require any finite-difference approximation of the boundary conditions.

Now, let us compare the DPM vs. BEM. The BEM is known as a numerical methodology for solving boundary integral equations of the classical potential theory. These boundary integral equations require knowing explicitly the fundamental solution of the corresponding differential operator; moreover, often these equations are not equivalent to the original boundary-value problem on the domain (e.g., the so-called "inner resonances" problem). The restrictions relevant to the equations of the classical potential theory are as well translated to the BEM. On the other hand, the pseudodifferential boundary equations known at the Calderon-Seeley equations require neither knowledge of the fundamental solutions nor use of the integrals. These equations are always equivalent to the original differential boundary-value problems on

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the domain. However, they cannot be discretized directly using any kind of numerical quadratures and/or BEM, because they do not contain any integrals at all. One possible viewpoint at the DPM is that it is a numerical methodology for solving the modified Calderon-Seeley equations. In this respect, the DPM plays the same role for the modified Calderon-Seeley boundary equations as the BEM does for the boundary integral equations of the classical potential theory.

There are also some similarities between the DPM and the capacitance matrix method [7], however these two methods actually employ difference potentials of different types.

Among the applications of the DPM we name the following:

- Numerical solution of internal and external boundary-value problems;
- Artificial boundary conditions for the numerical solution of infinite-domain problems;
- Domain decomposition, including some aspects of parallel computing;
- Finite-difference model for the problem of active shielding and noise control and its general solution.

2. Construction, Computation, and Properties of the Difference Potentials. The algorithm for constructing the difference potentials will be the following. First, we consider an arbitrary linear finite-difference equation or system on an arbitrary irregular grid and introduce a special grid contour and a piecewise-regular solution of the aforementioned equation/system with a discontinuity, i.e., jump, on this contour. Then, we show that for any prescribed jump there exists a unique piecewise-regular solution. Finally, the difference potential with the density from the space of jumps will be identified with the piecewise-regular solution, which has the same jump. This way of introducing the difference potentials is analogous to the well-known definition of the Cauchy-type integral:

$$(1) \quad u^\pm(z) = \frac{1}{2\pi i} \oint_{\Gamma} \frac{v_{\Gamma}(\zeta)}{\zeta - z} d\zeta,$$

which can be obtained as a piecewise-regular analytic function with the jump $v_{\Gamma}(\zeta)$ on the contour Γ and zero limit as $|z| \rightarrow \infty$.

Let us also note that the Cauchy-type integral can be interpreted as a potential for the Cauchy–Riemann system

$$(2) \quad \frac{\partial a}{\partial x} - \frac{\partial b}{\partial y} = 0, \quad \frac{\partial b}{\partial x} + \frac{\partial a}{\partial y} = 0,$$

that connects the real and imaginary parts of the analytic function

$$(3) \quad f(z) = a(x, y) + ib(x, y), \quad z = x + iy$$

that vanishes as $(x^2 + y^2) \rightarrow \infty$.

We will now give a rigorous definition of the difference potentials. Let M be an arbitrary finite set of points, we will call it the grid M ; and let $N_m, m \in M$, be another finite set of points (it may be different for different $m \in M$) that we will call the stencil of the finite-difference scheme centered at node $m \in M$. We define the grid $N = \bigcup_{m \in M} N_m$, and also introduce the coefficients $a_{mn}, m \in M, n \in N_m$, of the finite-difference equation. Finally, we specify some subspace U_N of the linear space W_N of all functions u_N defined on the grid N .

Then, we consider the equation with the coefficients a_{mn} :

$$(4) \quad \sum_{n \in N_m} a_{mn} u_n = 0, \quad m \in M,$$

and assume that the following problem

$$(5) \quad \sum_{n \in N_m} a_{mn} u_n = f_m, \quad m \in M$$

$$(6) \quad u_N \in U_N$$

has a unique solution u_N for every $f_M = \{f_m\}$, $m \in M$. The inclusion (6) can be considered a boundary condition for the equation (5). Here f_m , $m \in M$, and u_n , $n \in N$, can be vector-functions and a_{mn} , $m \in M$, $n \in N_m$, can accordingly be matrix coefficients.

DEFINITION 2.1. *Every function u_N , $u_N \in U_N$, is called a regular function.*

Let, for example, equation (4) be a standard five-point difference approximation of the Laplace equation on a Cartesian grid with the size $h = \frac{1}{K}$, where K is a positive integer. Let the grid M contain all the nodes $m = (m_1 h, m_2 h)$ which belong to the interior of the square $0 \leq x, y \leq 1$. Here, m_1 and m_2 are some integers.

Let the regular functions u_N from the space U_N satisfy the condition of vanishing at the sides of the square $0 \leq x, y \leq 1$. Then, the problem (5), (6) becomes a finite-difference counterpart to the Dirichlet problem for the Poisson equation. This problem has a unique solution for every right-hand side $f_M = \{f_m\}$. Moreover, this solution can be easily computed using the separation of variables (Fourier method).

Before proceeding any further, we note that all the constructions hereafter are valid for the general equations/systems (4), (5), (6), however, for the basic understanding of the methodology it is sufficient to conduct the analysis only for the foregoing example of the difference Poisson equation.

Let us now split the grid M into two arbitrary fixed subgrids M^+ and M^- , so that $M = M^+ \cup M^-$, $M^+ \cap M^- = \emptyset$. The system (4) is split accordingly into two subsystems:

$$(7) \quad \sum_{n \in N_m} a_{mn} u_n = 0, \quad m \in M^+,$$

$$(8) \quad \sum_{n \in N_m} a_{mn} u_n = 0, \quad m \in M^-.$$

The solutions of these subsystems are defined on the grids $N^+ = \bigcup_{m \in M^+} N_m$ and $N^- = \bigcup_{m \in M^-} N_m$, respectively.

DEFINITION 2.2. *The set $\gamma = N^+ \cap N^-$ is called a grid contour.*

DEFINITION 2.3. *Let $\xi_N^+ \in U_N$ and $\xi_N^- \in U_N$ be two arbitrary regular functions. We define the function u_N^\pm as*

$$(9) \quad u_n^\pm = \begin{cases} \xi_n^+, & \text{for } n \in N^+, \\ \xi_n^-, & \text{for } n \in N^-. \end{cases}$$

The function u_N^\pm is called a piecewise-regular function. Clearly, the function u_N^\pm of (9) has two values ξ_n^+ and ξ_n^- at every node $n \in \gamma$.

DEFINITION 2.4. The function v_γ defined on γ

$$v_\gamma|_n = \xi_n^+ - \xi_n^-, \quad n \in \gamma,$$

is called the jump $[u_N^\pm]_\gamma = v_\gamma$ of the piecewise-regular function u_N^\pm on the grid contour γ .

We will assume that the subdivision $M = M^+ \cup M^-$ is coherent with the choice of the space of regular functions U_N so that for every function $u_N \in U_N$ the following two functions

$$(10) \quad u_N^+ = \Theta_N(N^+)u_N, \quad u_N^- = \Theta_N(N^-)u_N$$

will also be regular, i.e., $u_N^+ \in U_N$, $u_N^- \in U_N$. Here $\Theta_Y(X)$ is an indicator of the subset $X \subset Y$. For the foregoing example (Laplace's equation) this requirement is satisfied for any subdivision $M = M^+ \cup M^-$.

Let us assume that a piecewise-regular function has the jump $v_\gamma = [u_N^\pm] = 0$, i.e., $\xi_n^+ = \xi_n^-$ for $n \in \gamma$. We will identify this piecewise-regular function u_N^\pm with the following single-valued function

$$(11) \quad u_N|_n = \begin{cases} \xi_n^+, & \text{for } n \in N^+ \setminus \gamma, \\ \frac{1}{2}(\xi_n^+ + \xi_n^-), & \text{for } n \in \gamma, \\ \xi_n^-, & \text{for } n \in N^- \setminus \gamma. \end{cases}$$

LEMMA 2.5. The single-valued function u_N defined (11) is regular, i.e., $u_N \in U_N$.

Proof. Clearly, the following equality

$$(12) \quad u_N = \Theta_N(N^+)\xi_N^+ + \Theta_N(N^-)\xi_N^- - \frac{1}{2}\Theta_N(N^+)\Theta_N(N^-)(\xi_N^+ + \xi_N^-)$$

is true. All three terms on the right-hand side of (12) are regular functions. Therefore, u_N is also a regular function, $u_N \in U_N$. \square

DEFINITION 2.6. The piecewise-regular function (9) is called a piecewise-regular solution to the equation (4) with boundary condition (6) if

$$(13) \quad \sum_{n \in N_m} a_{mn} \xi_n^+ = 0 \quad \text{for } m \in M^+,$$

$$(14) \quad \sum_{n \in N_m} a_{mn} \xi_n^- = 0 \quad \text{for } m \in M^-.$$

DEFINITION 2.7. Let u_γ be a function defined on γ such that $u_\gamma = u_N|_\gamma$, where $u_N \in U_N$. A space of all functions u_γ of this kind is called the space of jumps U_γ .

THEOREM 2.8. Let $u_\gamma \in U_\gamma$. A piecewise-regular solution u_N^\pm of problem (4), (6) with the jump v_γ exists and is unique. This piecewise-regular solution can be calculated by the formula

$$(15) \quad u_N^\pm = v_N^\pm - w_N,$$

where v_N^\pm is an arbitrary piecewise-regular function

$$(16) \quad v_N^\pm |_n = \begin{cases} v_N^+ |_n, & \text{for } n \in N^+, \\ v_N^- |_n, & \text{for } n \in N^-, \end{cases}$$

with the jump v_γ , and w_N is a solution to problem (5), (6) with the right-hand side given by

$$f_m = \begin{cases} \sum_{n \in N_m} a_{mn} v_N^+, & \text{for } m \in M^+, \\ \sum_{n \in N_m} a_{mn} v_N^-, & \text{for } m \in M^-. \end{cases}$$

Proof. Notice that a piecewise-regular function v_N^\pm with the jump v_γ exists for any given v_γ . In particular, the function (16), where

$$v_N^+ |_n = \begin{cases} 0, & \text{for } n \in N^+ \setminus \gamma, \\ v_\gamma |_n, & \text{for } n \in \gamma \end{cases},$$

$$v_N^- = 0, \quad \text{for } n \in N^-,$$

is one of such functions. Then, the regular function w_N can be identified with the following piecewise-regular function

$$w_N^\pm |_n = \begin{cases} w_N |_n, & \text{for } n \in N^+, \\ w_N |_n, & \text{for } n \in N^-, \end{cases}$$

which has two values at every node of γ but its jump is zero. Therefore, the function u_N^\pm defined by formula (15) has the same jump as the function v_N^\pm does, i.e., $[u_N^\pm]_\gamma = v_\gamma$. Furthermore, it is obvious that the function (15)

$$u_N^\pm |_n = \begin{cases} v_N^+ |_n - w_n & \text{for } n \in N^+, \\ v_N^- |_n - w_n & \text{for } n \in N^-, \end{cases}$$

solves equations (13), (14). This function is also a piecewise-regular solution of (4), (6) with the jump v_γ .

Let us now show that there is no other piecewise-regular solution \hat{u}_N^\pm to problem (4), (6) with the jump v_γ . Clearly, the piecewise-regular function $u_N^\pm - \hat{u}_N^\pm$,

$$(u_N^\pm - \hat{u}_N^\pm) |_n = \begin{cases} u_n^+ - \hat{u}_n^+ & \text{for } n \in N^+, \\ u_n^- - \hat{u}_n^- & \text{for } n \in N^-, \end{cases}$$

is a piecewise-regular solution with the jump $v_\gamma = 0$, i.e., it is a regular solution of problem (4), (6). However, this problem has only trivial solution, therefore

$$u_N^\pm = \hat{u}_N^\pm$$

□

DEFINITION 2.9. *The piecewise-regular solution u_N^\pm to problem (4), (6) with the jump $v_\gamma \in U_\gamma$ is called the difference potential*

$$(17) \quad u_N^\pm = P^\pm v_\gamma$$

with the density v_γ from the space of jumps.

REMARK 2.10. *We emphasize that neither the definition of the difference potential nor the algorithm for its calculation (Theorem 2.8) actually require knowledge of the fundamental solution or Green's function for problem (4), (6); therefore both the definition and the theorem are generic for the linear finite-difference systems.*

The difference potential $u^\pm = P^\pm v_\gamma$ is a piecewise-regular solution and consequently, it can be written in the form (9), (13), (14)

$$(18) \quad u_n^\pm = \begin{cases} u_n^+, & \text{for } n \in N^+, \\ u_n^-, & \text{for } n \in N^-. \end{cases}$$

We will also need the following notations:

$$(19) \quad \begin{aligned} u_n^+ &= P_n^+ v_\gamma, & \text{for } n \in N^+, \\ u_n^- &= P_n^- v_\gamma, & \text{for } n \in N^-. \end{aligned}$$

Let us now rewrite formula (17) as follows

$$(20) \quad u_n^\pm = \begin{cases} P_n^+ v_\gamma, & \text{for } n \in N^+, \\ P_n^- v_\gamma, & \text{for } n \in N^-. \end{cases}$$

DEFINITION 2.11. *The solution u_{N^+} (respectively, u_{N^-}) of equation*

$$(21) \quad \sum_{n \in N_m} a_{mn} u_n = 0 \quad \text{for } m \in M^+ \text{ (respectively, } m \in M^-)$$

defined on N^+ (respectively, N^-) is called a regular solution if there is a regular function $u_N \in U_N$ that coincides with u_{N^+} on $N^+ \subset N$ (respectively, $N^- \subset N$).

The properties of difference potentials established in Theorem 2.12 below constitute a foundation for all DPM-based algorithms.

THEOREM 2.12. *The function $v_\gamma \in U_\gamma$ can be complemented on N^+ to a regular solution v_{N^+} of equation (21) if and only if the equality*

$$(22) \quad P_n^+ v_\gamma = v_n \quad \forall n \in \gamma$$

holds. If equality (22) holds, then the complement is unique. It coincides with the difference potential

$$(23) \quad v_n = P_n^+ v_\gamma \quad \text{for } n \in N^+.$$

Proof. Let the function $v_\gamma \in U_\gamma$ satisfy equality (22). Then the regular solution v_{N^+} defined by formula (23) coincides with v_γ on γ .

Conversely, let the function v_γ be such that there is a complement v_{N^+} that is a regular solution of equation (21) on N^+ . Then the piecewise-regular function

$$\hat{u}_n^\pm = \begin{cases} v_n, & \text{for } n \in N^+, \\ 0_n, & \text{for } n \in N^- \end{cases}$$

is actually a piecewise-regular solution of equation (4) with the jump

$$[\hat{u}^\pm]_\gamma = v_\gamma - 0_\gamma = v_\gamma,$$

i.e., the function \hat{u}^\pm is a difference potential with the density v_γ . Therefore, the function v_{N^+} is unique, namely, it can be represented as

$$(24) \quad v_n = P_n^+ v_\gamma \quad \text{for } n \in N^+.$$

Formula (24) is the same as formula (23). \square

3. DPM-based Numerical Algorithms. We are going to illustrate some key ideas of the algorithms using the Laplace equation

$$(25) \quad \frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} = 0, \quad (x, y) \in D.$$

We assume that the closure \bar{D} of domain D belongs to the interior of the unit square $0 < x, y < 1$. We will use the aforementioned five-point difference analogue of the Laplace equation. Let M^+ be a set of all grid nodes m , $m \in \bar{D}$. Then, M^-, N^+, N^- , and $\gamma = N^+ \cap N^-$ are determined automatically in accordance with the foregoing constructions. Let $u(x, y)$ be a sufficiently smooth function defined on some domain Q such that Q contains both \bar{D} and N^+ . Let u_{N^+} be a trace of $u(x, y)$ on N^+ , i.e., $u_n = u_{N^+}|_n$ coincides with $u(x, y)$ at the nodes n , $n \in N^+$. Clearly, the function u_{N^+} is an approximate solution to the finite-difference analogue of the Laplace equation (25). Therefore, equalities (22) and (23), i.e.,

$$(26) \quad P_n^+ u_\gamma = u_n, \quad n \in \gamma$$

$$(27) \quad P_n^+ u_\gamma = u_n, \quad n \in N \supset \gamma$$

are approximately satisfied as well.

Having made these comments, we will now consider the following three problems.

3.1. Boundary-value Problem. Let the Laplace equation (25) be supplemented by the Dirichlet boundary condition

$$(28) \quad u(x, y)|_\Gamma = \varphi(s), \quad (x, y) \in \Gamma$$

where $\varphi(s)$ is a given function of the arc length s on the curve $\Gamma = \partial D$. Let the equality

$$(29) \quad \frac{\partial u(x, y)}{\partial n} \Big|_\Gamma = \sum_{l=1}^L C_l' \psi_l(s)$$

be an approximation of the normal derivative of the solution $u(x, y)$ on Γ in the interior direction; here $C'_l(s)$, $l = 1, 2, \dots$, are some (undetermined) coefficients. We assume that as the number of terms L in the sum (29) increases, the accuracy of approximation for the normal derivative improves as well. We will define the function v_γ at any node $\nu \in \gamma$ using Taylor's expansion:

$$(30) \quad v_\nu = \varphi(s_\nu) + \rho_\nu \sum_{l=1}^L C_l \psi_l(s_\nu),$$

where s_ν is the foot of the normal dropped from the node $\nu \in \gamma$ to the curve Γ and ρ_ν is the distance between $\nu \in \gamma$ and $s = s_\nu \in \Gamma$. The sign of ρ_ν is positive if $\nu \in \bar{D}$ and negative if $\nu \notin \bar{D}$. If the coefficients C'_1, C'_2, \dots, C'_L were known, then the function (30)

$$(31) \quad v_\gamma = v_\gamma(C'_1, C'_2, \dots, C'_L)$$

could have been plugged into equation (26) and would have actually been its approximate solution, i.e.,

$$(32) \quad P_\gamma^+ v_\gamma = v_\gamma.$$

As C'_l are unknown, equality (32) can be used for determining these coefficients. The system of linear equations (32) with respect to C'_l may be overdetermined; then, we will be looking for its solution C'_1, C'_2, \dots, C'_L in the sense of least squares.

After the coefficients C'_1, C'_2, \dots, C'_L have been found, the approximate solution $u(x, y)$ of (25), (28) can be represented as

$$u_n \approx P_n^+ v_\gamma, \quad n \in N^+.$$

We do not delineate here what specific Euclidean norm should be chosen for the method of least squares.

3.2. Superelement. Following the foregoing algorithm we can construct an approximate solution of the Laplace equation (25):

$$(33) \quad u(x, y) = u(x, y, C_1, C_2, \dots, C_R),$$

which will depend on the set of arbitrary parameters C_1, C_2, \dots, C_R ; R is some positive integer. Under the proper choice of these parameters, the solution (33) can approximate any particular solution of the Laplace equation $u(x, y)$ and the corresponding approximation error will vanish as $R \rightarrow \infty$.

Formula (33) can be rewritten in the form

$$(34) \quad u(x, y) = \sum_{r=1}^R C_r u_r(x, y),$$

where $u_r(x, y)$ is a solution to the Dirichlet problem (25), (28) with

$$(35) \quad \varphi(s) = \psi_r(s), \quad r = 1, 2, \dots, R.$$

Let now the grid size h approach zero, $h \rightarrow +0$, and $L \rightarrow \infty$ (see formula (30)), $R \rightarrow \infty$. Then, formula (34) will approximate any particular solution $u(x, y)$ of the Laplace equation (25). In this respect, formula (34) yields an approximate general solution to the Laplace equation.

REMARK 3.1. *We emphasize that no finite-difference approximation to the boundary conditions (28) and (35) has been used.*

3.3. Domain Decomposition. Let us consider a problem formulated on a domain of complex shape; in addition, the gradient of the solution may vary strongly across the domain. Let then split the domain into a number of appropriate subdomains and construct a superelement of type (34) on each subdomain. Different independent grids and different problems similar to (5), (6) can be used for constructing each of these superelements. Therefore, one can calculate all the superelements independently and possibly, concurrently, which is well suited for parallel implementation. After the superelements have been constructed, we choose the parameters C_1, C_2, \dots, C_R so that to satisfy the boundary conditions and matching conditions on interfaces between the superelements.

3.4. Auxiliary Problem and Its Choice. The difference potential

$$P_n^+ v_\gamma = u_n, \quad \text{for } n \in N^+,$$

depends on the choice of problem (5), (6). However, the possibility to complement v_γ everywhere on N^+ to a regular solution of the equation

$$\sum_{n \in N_m} a_{mn} u_n = 0, \quad \text{for } m \in M^+.$$

does not depend on such changes of M, N_m, a_{mn}, U_N that would leave the sets M^+, N^+, γ, a_{mn} , and N_m for $m \in M^+$, as well as the set of all regular solutions on N^+ , unaltered. Therefore, the class of all functions satisfying equality (22) is not affected by the changes of this type as well. Hence, we do have a certain flexibility in choosing the problem (5), (6), if we eventually need only to meet the condition (22). In this case, the problem (5), (6) can be considered an auxiliary problem for satisfying (22). One can choose an appropriate auxiliary problem to make the actual computation of the difference potential

$$u_n = P_n^+ v_\gamma, \quad n \in N^+$$

easy and convenient, which is important for implementation.

4. Brief Bibliographical Survey.

- Apparatus of the DPM: [9, 11, 13].
- Discretization and numerical solution of the Calderon-Seeley boundary equations: [8, 11, 13, 16].
- Artificial boundary conditions for the numerical solution of infinite-domain problems: [2, 14, 20, 23, 24].
- Implementation of the DPM for domain decomposition algorithms: [4, 5, 10, 16].
- Problems with complex boundary conditions, e.g., a viscous flow problem in the vorticity–stream function formulation: [19].
- Active shielding and noise control: [15, 17, 21].

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