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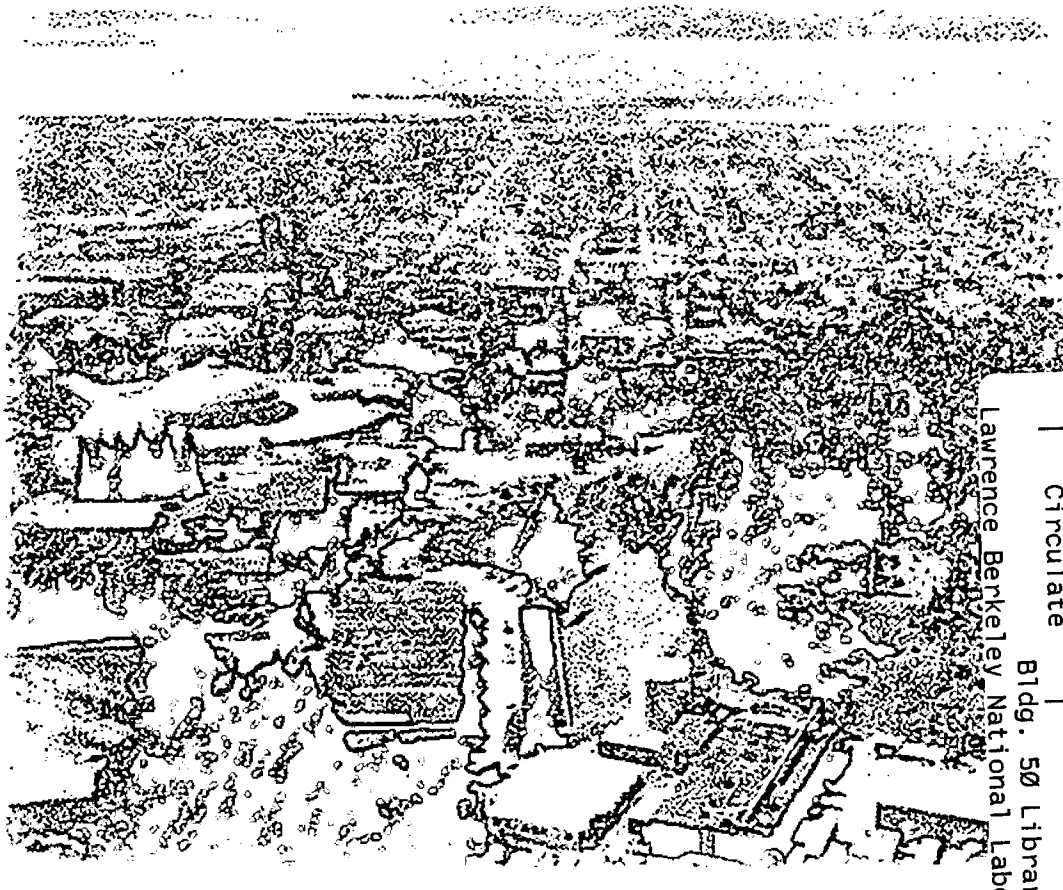

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The Explicit Jump Immersed Interface Method and Integral Formulas[1]

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Abstract

The well known discretization of the Dirichlet boundary condition for the Laplace equation on a rectangle is shown to be a special case of the Explicit Jump Immersed Interface Method. For one-dimensional boundary value problems, Schur–complements for finite difference discretizations are pointwise discretizations of integral formulas. The analogy requires a discretization of the delta and dipole, which may occur even on the domain boundary.

1 Introduction

The Explicit Jump Immersed Interface Method (EJIIM) is a finite difference method for the approximation of discontinuous or non–differentiable solutions to differential equations (DE). These may arise from singularly supported sources in the equation, from embedding the domain of interest in a larger domain which allows fast numerical solutions, or from discontinuities in the coefficients of the differential equation. We focus here on the first two situations, the last case is treated in [1] and [10].

We study the one-dimensional "Singular Poisson Equation" and one-dimensional Boundary Value Problems (BVP) for the purpose of simplifying access to our work on elliptic problems in higher dimensions and consider one-dimensional problems for two reasons. In 1D, the Connections between the discretization of the DE and integral equations are simple and exact while in higher dimensions insights from potential theory are required and the discretizations are only approximate. Secondly, the treatment of discontinuities in solutions and their derivatives is much simpler in 1D, because of the simple one-point structure of boundaries and interfaces. Except for these simplifications, the EJIIM is the same in higher dimensions.

We will illustrate several aspects of the EJIIM with simple examples.

1. *Integral equation interpretation of well-known discretization approaches.*
2. *Irregularity of the discrete solution of an elliptic differential equation.*
3. *Preconditioning a discretized DE by a fast solver and integral formulas.*
4. *Schur–complements and Boundary Integral formulas.*

To emphasize the introductory nature of this work, we have included exercises that enable the readers to immediately test their understanding of the material.

2 Poisson problem, Green's kernel and their discretizations

2.1 A 1D Poisson problem

Let f in $C^1(0,1)$. Consider the 1D Poisson problem

$$\begin{aligned} u_{xx} &= f, \\ u(0) &= 0, \\ u(1) &= 0. \end{aligned} \tag{1}$$

We integrate f, determine the two constants of integration and see that it is solved by

$$\begin{aligned} u(x) &= \int_0^x \int_0^y f(\xi)d\xi dy - x\left(\int_0^1 \int_0^y f(\xi)d\xi dy\right) \\ &= \int_0^x (x-y)f(y)dy - x\int_0^1 (1-y)f(y)dy \\ &= \int_0^x (x-y)f(y)dy - \int_0^x x(1-y)f(y)dy - \int_x^1 x(1-y)f(y)dy \\ &= \int_0^x (x-1)yf(y)dy + \int_x^1 (y-1)xf(y)dy \\ &= \int_0^1 G(x,y)f(y)dy, \text{ for } x \in [0,1]. \end{aligned} \tag{2}$$

Here, the *Green's kernel*[1] for the interval $[0,1]$ is

$$G(x,y) = \begin{cases} (x-1)\,y & 0 \le y \le x \le 1, \\ (y-1)\,x & 0 \le x \le y \le 1. \end{cases} \tag{3}$$

[1]This is an unfortunate misnomer because it really is the kernel for the Poisson problem, and should be called Poisson kernel — but this name is reserved for the kernel for the Dirichlet problem!

We view integration against the Green's kernel (3) as a global operation that solves the differential equation (1) with boundary conditions*by inverting the differential operator including boundary conditions.*

2.2 The discrete 1D Poisson problem

The usual centered finite differences

$$\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} = f_i \tag{4}$$

are used in the discretization of (1) on equidistant interior grid points $x_i = ih$, $i = 1, 2, \ldots, n-1$, with $h = 1/n$. When $u_{xx} = f$ is differentiable, the truncation error is seen via Taylor expansions to be

$$T_i = f(x_i) - \frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{h^2} = O(h^2)\,. \tag{5}$$

For the two interior points next to the boundary, we use the boundary conditions $u(0) = u_0 = 0$ and $u(1) = u_1 = 0$ and find

$$\begin{aligned} u_{xx}(h) &= \frac{0 - 2u(h) + u(2h)}{h^2} + O(h^2)\,, \\ u_{xx}(1-h) &= \frac{u(1-2h) - 2u(1-h) + 0}{h^2} + O(h^2)\,. \end{aligned}$$

Writing (4) in matrix form, the Poisson problem is discretized as

$$\mathcal{A}U = F. \tag{6}$$

For example, on the grid with $h = 1/4$, i.e. on the points $\{0, 0.25, 0.5, 0.75, 1\}$, the differential operator ∂_{xx} including the boundary conditions $u(0) = u(1) = 0$ is discretized by the matrix

$$\mathcal{A}_3 = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}$$

The entries in U approximate the solution at the interior points $\{0.25, 0.5, 0.75\}$ and $F = [f(0.25), f(0.5), f(0.75)]^T$ approximates the right hand side. In general, for Dirichlet boundary conditions, the discrete solution lives on the $n-1$ interior points of the discretization of $[0,1]$ by n intervals with $h = 1/n$. We will see in §4 that problems with non-vanishing Dirichlet boundary data are numerically approximated *by the same matrix* $\mathcal{A}$ as Poisson problems, but with singular right hand side.

2.3 Connection between the discretization of the differential equation and the integral formula

The matrix $\mathcal{A}$ is tridiagonal, and U can be found in $\mathcal{O}(n)$ operations. In higher dimensions, this is not the case and we turn to fast solvers in Fourier space (Fast Poisson solvers, [8]) instead. From [10, 7] we know

Lemma 1 *The (i,j) entry of* $\mathcal{A}^{-1} \in \mathbf{R}^{(n-1)\times(n-1)}$ *(for* $n > 3$*) is*

$$a_{ij} = \frac{\min(i,j)\,(\max(i,j) - n)}{n^3}.$$

For the above example this gives

$$\mathcal{A}^{-1} = -\frac{1}{64}\begin{pmatrix} 3 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 3 \end{pmatrix}.$$

Also from [10, 7], we know that

Lemma 2 $\|\mathcal{A}^{-1}\|_\infty = \frac{1}{8}$ *for n even and* $\|\mathcal{A}^{-1}\|_\infty = \frac{1-n^{-2}}{8}$ *for n odd.*

This uniform boundedness of the inverse operator, together with the second order consistency of the discretization, combine to give second order convergence. The solution to the discrete problem is

$$U = \mathcal{A}^{-1}F, \tag{7}$$

The evaluation of the true solution on the grid points (denoted by Eu) satisfies

$$Eu = \mathcal{A}^{-1}(F - T). \tag{8}$$

where the norm of the truncation error is $\|T\|_\infty = O(h^2)$. Hence $\|U - Eu\|_\infty = \|\mathcal{A}^{-1}T\|_\infty \leq \|\mathcal{A}^{-1}\|_\infty \|T\|_\infty = O(h^2)$, and we have proved the following theorem.

Theorem 3 *As the grid is refined, the solution to the discretized problem converges in the infinity norm on grid points with second order to the solution of the differential equation.*

The main point of this § is the analogy between (7) and (2). The entries of $\mathcal{A}^{-1}$ in (1) are equal to values of the Green's kernel (3) at the grid points, multiplied by h; this factor h corresponds to *integration* against the kernel. **Instead of viewing (6) as discretizing the differential equation (1), we view the system (7) as discretizing the Green's kernel-based integral formula (2). Finite difference operators discretize differential operators including boundary conditions, and their inverses may approximate integral formulas!**

3 Known discontinuities in the solution to a Poisson Equation

3.1 Differential equations with singular sources

Since the EJIIM deals with discontinuities in solutions of differential equations (or discontinuities in their derivatives), it is essential to have a good understanding of the *delta* and *dipole* (also called *doublet*). These distributions introduce irregularity into the solution of the Poisson equation when placed on the right hand side.

Definition 1 (1D delta, dipole) *Let* $\gamma \in (0, 1)$.
The **delta** $\delta(x-\gamma)$ *(centered at* γ*) is the distribution that satisfies* $\int_0^1 \Phi(x)\delta(x-\gamma)dx = \Phi(\gamma)$ *for any function* $\Phi \in C^\infty([0,1])$.
The **dipole** $\delta'(x-\gamma)$ *(centered at* γ*) is the distribution that satisfies* $\int_0^1 \Phi(x)\delta'(x-\gamma)dx = -\Phi'(\gamma)$ *for any function* $\Phi \in C^\infty([0,1])$.

Definition 1 gives mathematically precise meaning, while the following aspects are also important for understanding EJIIM.

1. *The delta and dipole are convenient short notation for the fact that a solution to a differential equation has a discontinuous derivative, or is discontinuous itself.* This view will allow us to apply the standard "integration against a kernel" approach to find solutions to the differential equation.

2. *The delta and dipole can be viewed as "singular" limits of certain C^∞ functions with fixed L^1 norm as their support vanishes.* This view helps interpret our discretization of the differential equation.

3. *The delta and dipole are useful for making sense of* integration by parts, *an essential tool for differential equations.* This view will initially be least useful for EJIIM, but is the most easily appreciated interpretation. Later, we will see a correspondence between integration by parts (Green's identities) on the differential equation side and Schur complements on the discretized equation side.

An immediate benefit of introducing the delta is the characterization of the Green's kernel in a form that carries over to higher dimensions. The importance of the formula (2) for the solution of the Poisson problem lies in the fact that it is valid even for singular (distributional) right hand side f and that ot carries over

verbatim to higher dimensional Poisson problems, at least for sufficiently nice domains. In 1D, the Green's kernel satisfies $\partial^2 G(x,y)/\partial x^2 = \delta(x-y)$ with $G(0,y) = G(1,y) = 0$ for all $y \in (0,1)$. It is symmetric and negative everywhere in $(0,1) \times (0,1)$. In higher dimensions, too, there exists a unique G defined by just the above properties: It satisfies a Poisson equation with a delta on the right hand side, vanishes on the boundaries, is symmetric in x and y, and is negative where finite.

Consider the integral formula (2) for the Poisson problem with the following four increasingly singular right hand sides. The irregularity occurs always at the same point $\alpha \in (0,1)$; by 1_Ω we mean the characteristic function of the set Ω.

1. $f = (x-\alpha)1_{\{\alpha<x<1\}}$ (f continuous but not differentiable)
2. $f = 1_{\{\alpha<x<1\}}$ (f discontinuous)
3. $f = \delta(x-\alpha)$ (f first order singular)
4. $f = \delta'(x-\alpha)$ (f second order singular)

For all 4 cases, the solution via (2) makes sense. The reader is asked to convince herself (see Exercise 3.3) that these solutions satisfy the differential equation in the classical sense away from α, while becoming more and more singular at α. Technically, G does not satisfy the requirements on the test function Φ in the definitions of the delta and dipole. The biggest problem occurs in applying the dipole at the kink of G, where the derivative does not exist. However, for any $u(\alpha)$ the solution

$$u(x) = \int_0^1 G(x,y)\delta'(y-\alpha)dy = -\frac{\partial G}{\partial y}(x,\alpha) = \begin{cases} -x & x<\alpha, \\ u(\alpha) & x=\alpha, \\ 1-x & \alpha<x, \end{cases}$$

is conceivable, with $u(\alpha) = 1/2 - \alpha$ most satisfactory because it it has the property that values of u are the averages of one-sided limits. For continuous f, we find that $u \in C^2$; for discontinuous f, we get $u \in C^1$; for first order singular f, we get $u \in C^0$ and for second order singular f, we get $u \in H^1$, the subspace of functions in L^2 whose derivative is also in L^2. In all cases, only one of the derivatives of u is discontinuous[2], and the magnitude of the jump[3] is 1.

Exercise 3.1 *Verify in one space dimension that $G(x,y) = N(y-x) + H(x,y)$, where N is the fundamental solution (Newtonian potential) that satisfies $\Delta N = \delta(x)$ and H is a harmonic (in 1D, that means affine) function in x for every y which is introduced to achieve the desired boundary values: $H(0,y) = -N(y)$ and $H(1,y) = -N(y-1)$.*

Hints: Your solution G has to agree with (3). Usually the fundamental solution is made unique by specifying its asymptotic behavior near infinity. For the (nonstandard) N in 1D, we require $\inf(N) = 0$.

3.2 EJIIM for singular sources

The conceptually easiest application of EJIIM is the numerical approximation of problems with right hand sides of the type 1-4. This is the context in which Li and LeVeque's Immersed Interface Method [1, 2] is preceded by Peskin's Immersed Boundary Method [4] and Mayo's Fast Poisson solvers on irregular domains [3]. The EJIIM formulas from [10, 7] deal with two issues at the same time:

1. The truncation error in (4) deteriorates as u becomes less smooth.
2. We need to discretize singular f.

The idea is to use the knowledge of the irregularity of u introduced by f (as given by the integral formula) and to build it into the discretization. The strength of the dipole is the jump in u, the strength of the delta is the jump in u_x, the jump in f is the jump in u_{xx}, the jump in f_x is the jump in u_{xxx} and so

[2] By convention, u is its own zeroth derivative.

[3] From a practical point of view, the search for non-smooth solutions of the PDE with prescribed jumps is the reason to study singular f.

forth. This results simply in "corrections" to the standard formulas applicable on the right hand side of the discretization (4) for the smooth case; these corrections may be viewed as a discretization of the singularity of f. Contributions of different singularity are each separated into the strength of the discontinuity and the discretization of the normalized singularity, i.e. how it influences the solution on the grid.

In this sense we will speak of grid functions resulting from discretizations of second order PDE as "differentiable", "not differentiable" and "discontinuous" between grid points if the right hand side for the two neighboring grid points behaves under refinement like $\mathcal{O}(1)$) (i.e. is a function), $\mathcal{O}(h^{-1})$) (i.e. is first order singular) and $\mathcal{O}(h^{-2})$) (i.e. is second order singular), respectively.

We copy the main result on how to do this from [10] as Lemma 4. Square brackets $[u^{(m)}] = u^{(m)}(\alpha^+) - u^{(m)}(\alpha^-)$ indicate jumps, i.e. the difference subtracing the left limit of u at the point α from the right limit.

Lemma 4 (jump-corrected differences) *Let $x_j \le \alpha < x_{j+1}$, $h^- = x_j - \alpha$ and $h^+ = x_{j+1} - \alpha$. Suppose $u \in C^4[x_j - h, \alpha) \cap C^4(\alpha, x_{j+1} + h]$, with derivatives extending continuously up to the boundary α. Then the following approximations hold to $O(h^2)$:*

$$u_x(x_j) \approx \frac{u(x_{j+1}) - u(x_{j-1})}{2h} - \frac{1}{2h}\sum_{m=0}^{2} \frac{(h^+)^m}{m!}[u^{(m)}],$$

$$u_x(x_{j+1}) \approx \frac{u(x_{j+2}) - u(x_j)}{2h} - \frac{1}{2h}\sum_{m=0}^{2} \frac{(h^-)^m}{m!}[u^{(m)}],$$

$$u_{xx}(x_j) \approx \frac{u(x_{j+1}) - 2u(x_j) + u(x_{j-1})}{h^2} - \frac{1}{h^2}\sum_{m=0}^{3} \frac{(h^+)^m}{m!}[u^{(m)}], \tag{9}$$

$$u_{xx}(x_{j+1}) \approx \frac{u(x_{j+2}) - 2u(x_{j+1}) + u(x_j)}{h^2} + \frac{1}{h^2}\sum_{m=0}^{3} \frac{(h^-)^m}{m!}[u^{(m)}]. \tag{10}$$

The system (6) becomes

$$\mathcal{A}U = F + \Psi C \tag{11}$$

where $C \in \mathbf{R}^4$ is the vector of jump strengths $\{[u], [u_x], [u_{xx}], [u_{xxx}]\}$as in Lemma 4, and $\Psi \in \mathbf{R}^{n-1} \times \mathbf{R}^4$ has two non-zero entries per column, introducing the jumps in C into the jth and $(j+1)^{st}$ equations with the correct geometry. For example the first column corresponds to $[u]$ and has non-zero entries $\Psi(1,j) = 1/h^2$ and $\Psi(1,j+1) = -1/h^2$. In exercise 3.4 the reader is asked to show that Theorem 3 still holds for this singular case and even if the corrections are used only up to $[u_{xx}]$.

Exercise 3.2 *Plot $\Psi(1,\cdot)$ and $\Psi(2,\cdot)$ for fixed α, $x_j \le \alpha < x_{j+1}$, as $n \to \infty$ to get a geometric intuition of the discrete dipole $\Psi(1,\cdot)$ and the discrete delta $\Psi(2,\cdot)$.*

Exercise 3.3 *a) Find the solutions to problem (1) with f given by*

1. $f = (x-\alpha)1_{\{\alpha<x<1\}}$,
2. $f = 1_{\{\alpha<x<1\}}$,
3. $f = \delta(x-\alpha)$,
4. $f = \delta'(x-\alpha)$.

b) Verify that knowledge of the jumps in u and jumps in its derivatives and discretization via Lemma 4 leads to a pointwise recovery of the solutions from part a) for any uniform mesh.

Exercise 3.4 *a) Given right hand side f that is smooth except for singularities up to second order at a finite number of points, show that using (9) and (10), the discrete solutions to (1) converge to the solution of the continuum problem like $O(h^2)$ in the maximum norm on grid points.*

Hint: The discretized integration against the kernel smoothes the truncation error by one order. Adjust the proof for the more difficult discontinuous coefficient case from [10]. *b) Show that the result in a) holds even if the $[u_{xxx}]$ terms are dropped from (9) and (10).*

4 Dirichlet BVP via Poisson Problem

4.1 A 1D Dirichlet problem

Let u_0 and $u_1 \in \mathbf{R}$, and consider the Dirichlet BVP:

$$u_{xx} = 0 \quad \text{in } (0,1), \tag{12}$$
$$u(0) = \bar{u}_0, \tag{13}$$
$$u(\alpha) = \bar{u}_1. \tag{14}$$

First consider the case $\alpha = 1$. Existence and uniqueness of the solution of this problem are trivial,

$$u(x) = \bar{u}_0 + x\,(\bar{u}_1 - \bar{u}_0), \text{ for } x \in [0,1]. \tag{15}$$

There exists another important way to write the solution, which is analoguous to standard boundary integral methods in higher dimensions:

$$u(x) = -\frac{\partial}{\partial y}G(x,y)\bigg|_{y=0} \bar{u}_0 + \frac{\partial}{\partial y}G(x,y)\bigg|_{y=1} \bar{u}_1. \tag{16}$$

The kernel here, *the outward normal derivative of the Green's kernel along the boundary*, is known as the *Poisson kernel* in higher dimensions. We need to interpret (16) for $x = 0$ and $x = 1$, because in these cases the derivatives at $y = 0$ and $y = 1$, respectively, do not exist. However, both one sided limits for the derivatives of G exist in both cases, and taking the limits for $y \in (0,1)$ yields exactly (15), while applying the limits for $y \notin (0,1)$ results in $u(0) = u(1) = 0$.

We choose to write the solution in the following peculiar form, using the solution for a *Poisson problem* by integration against the Green's kernel (2) to solve a *Dirichlet problem*!

$$\begin{aligned} u(x) &= \lim_{\epsilon \to 0+} \int_0^1 G(x,y)\,(u_0\delta'(y-\epsilon) - u_1\delta'(y-(1-\epsilon)))\,dy = \\ &= \lim_{\epsilon \to 0+} \int_0^1 G(x,y)\,([u]_0\delta'(y-\epsilon) + [u]_1\delta'(y-(1-\epsilon)))\,dy, \text{ for } x \in (0,1). \end{aligned} \tag{17}$$

The sole purpose of the limit in this formula is to define the application of δ' to G at a point of discontinuity by using a one-sided limit. On the boundary, i.e. for $x \in \{0,1\}$, (17) **does not agree** with (15). The function defined by (17) on $[0,1]$ has jumps $[u]_0 = u_0$ and $[u]_1 = -u_1$ at the left and right endpoints, respectively!

4.2 The discrete 1D Dirichlet problem

Consider again $n = 4$, discretize the differential operator on interior points as for the Poisson problem, and the boundary condition at the boundary points.

$$\frac{1}{h^2}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} = \begin{pmatrix} \bar{u}_0/h^2 \\ 0 \\ 0 \\ 0 \\ \bar{u}_1/h^2 \end{pmatrix} \tag{18}$$

Elimintion of known variables is the easiest example of a Schur–complement and yields

$$\mathcal{A}_3 U = \left(-\frac{1}{h^2}\begin{pmatrix} \bar{u}_0 \\ 0 \\ \bar{u}_1 \end{pmatrix}\right). \tag{19}$$

The solution to our discrete model problem on $\{0, 0.25, 0.5, 0.75, 1\}$ is

$$U = \mathcal{A}_3^{-1}\left(-\frac{1}{h^2}\begin{pmatrix} \bar{u}_0 \\ 0 \\ \bar{u}_1 \end{pmatrix}\right) = \mathcal{A}_3^{-1}\begin{pmatrix} -[u]_0/h^2 \\ 0 \\ [u]_1/h^2 \end{pmatrix}, \tag{20}$$

which results from simply moving the known boundary values in the discretization of the Laplacian (4) onto the right hand side. The standard way of solving the Dirichlet problem (20) discretizes (17) just as (7) discretizes (2). Also, (20) is a special case of (9) and (10) in the following sense:

Consider $x_{n-1} \leq \alpha < 1$, and recall that the discretization of the Poisson problem $\mathcal{A}$ imposes $u(1) = 0$ on the discretization. Equation (9) in this case is

$$u_{xx}(x_{n-1}) \approx \frac{0 - 2u(x_{n-1}) + u(x_{n-2})}{h^2} - \frac{1}{h^2} \sum_{m=0}^{3} \frac{(1-\alpha)^m}{m!} [u^{(m)}]_1. \tag{21}$$

In the limit as $\alpha \longrightarrow 1$, this becomes

$$\begin{aligned} u_{xx}(x_{n-1}) &\approx \frac{-2u(x_{n-1}) + u(x_{n-2})}{h^2} - \frac{1}{h^2} \sum_{m=0}^{3} \frac{0^m}{m!} [u^{(m)}]_1 = \\ &= \frac{-2u(x_{n-1}) + u(x_{n-2})}{h^2} - \frac{[u]_1}{h^2}. \end{aligned}$$

So $u_{xx}(x_{n-1}) = 0$ and $u(1) = 0$ becomes

$$\frac{-2u_{n-1} + u_{n-2}}{h^2} = \frac{[u]_1}{h^2}$$

just as in (20). The question now becomes: What is the continuous equation discretized by (4), modified to (21) at x_{n-1}?

4.3 Connection between the discretization of the differential equation and an integral formula

The answer depends on what we use for $[u_x]$, $[u_{xx}]$ and $[u_{xxx}]$. For example, $[u_{xx}] = [f]$ and $[u_{xxx}] = [f_x]$ depend on the extension of f to $(\alpha, 1)$. For $f = 0$ on$(0, \alpha)$ the extensio is zero, and $[u_{xx}] = [u_{xxx}] = 0$; but in any case, $[u_{xx}]$ and $[u_{xxx}]$ can be known from the problem data. The choice of $[u_x]$ has a bigger impact. For EJIIM, we propose $[u_x] = -u_x^-$, while the earlier capacitance matrix approach [5] as incorporated into the IIM [11] used $[u_x] = 0$. In the first case, $[u_x]$ needs to be determined as part of the solution; in the second case, $[u_x]$ is known. This seeming disadvantage of the EJIIM is outweighed by the fact that for this choice of $[u_x]$ together with always extending f by 0 on $(\alpha, 1)$, the extension of u by zero $(\alpha, 1)$ satisfies all jump conditions and boundary conditions as well as the extension of the differential equation, and is the unique solution to $u_x(\alpha) = 0$, $u(1) = 0$, $u_{xx}(x) = 0$ in $(\alpha, 1)$, where the first boundary condition follows from $[u_x] = u_x^- \Rightarrow u_x^+ = 0$. Finally, $u \equiv 0$ on $(\alpha, 1)$ and $[u]_\alpha = -\bar{u}_1$ guarantees $u^-(\alpha) = \bar{u}_1$. In the capacitance matrix approach, the correct boundary limit $u(1)$ needs to be found and f needs to be extended differentiably in order to make $u^+(\alpha) = 0$.

By D^T_{x,α^-} we denote the unique linear operator that extrapolates the derivatives of a grid function at α, based on the three grid points to the left of α, to second order. The EJIIM for (12)–(14) can be written as

$$\begin{aligned} \mathcal{A}U &= \frac{1}{h^2} \begin{pmatrix} -[u]_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \frac{(1-\alpha)}{h^2} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ C \end{pmatrix}, \\ C &= -D^T_{x,\alpha^-} U. \end{aligned}$$

Shortening D^T_{x,α^-} to D^T and writing $\tilde{F} = (-[u]_0, 0, \ldots, 0)/h^2$ and $\Psi_1 = \left(0, 0, \ldots, (1-\alpha)/h^2\right)^T$, this is

$$\begin{aligned} \mathcal{A}U &= \tilde{F} + \Psi_1 C, \\ C &= -D^T U. \end{aligned}$$

The first set of equations includes (18)! We rewrite it:

$$U = \mathcal{A}^{-1}(\tilde{F} + \Psi_1 C),$$

and form the Schur complements for the variables U and C:

$$(I + \mathcal{A}^{-1}\Psi_1 D^T)U = \mathcal{A}^{-1}\tilde{F}, \tag{22}$$

$$(I + D^T\mathcal{A}^{-1}\Psi_1)C = -D^T\mathcal{A}^{-1}\tilde{F}. \tag{23}$$

Equations (22) and (23) are discretizations of the two integral equations that appear in the following Lemma.

Lemma 5 *The solution to the problem (12)–(14) and the jump $c = [u_x] = -u_x^-(\alpha)$ satisfy*

$$u(x) + \int_0^1 G(x,y)\delta(y-\alpha)\frac{d}{dx}u(x)\Big|_{x=\alpha^-} dy = \int_0^1 G(x,y)\left\{\delta'(y-\alpha)u_1 + \delta'(y-0)u_0\right\} dy, \tag{24}$$

$$c + \frac{d}{dx}\int_0^1 G(x,y)\delta(y-\alpha)c\, dy\Big|_{x=\alpha^-} = -\frac{d}{dx}\int_0^1 G(x,y)\left\{\delta'(y-\alpha)u_1 + \delta'(y-0)u_0\right\} dy\Big|_{x=\alpha^-}. \tag{25}$$

Proof. (25) follows immediately from (24) by applying $\frac{d}{dx}(\cdot)\big|_{x=\alpha^-}$ to both sides and renaming $c = \frac{d}{dx}(u)\big|_{x=\alpha^-}$, just as in the discrete case. To see that u must satisfy (24), we decompose $u = u_0 + [u_x]u_1 + [u]u_2$, where

$$\begin{array}{lllllllll}
\Delta u_0 & = & 0 & \text{with} & u_0(0) & = & \bar{u}_0, & u_0(1) & = & 0, \\
\Delta u_1 & = & \delta(x-\alpha) & \text{with} & u_1(0) & = & 0, & u_1(1) & = & 0, \\
\Delta u_2 & = & -\delta(x-\alpha) & \text{with} & u_2(0) & = & 0, & u_2(1) & = & 0,
\end{array}$$

satisfy

$$u_0(x) = \int_0^1 G(x,y)(-\bar{u}_0)\delta'(y-0)dy = \begin{cases} 0 & x = 0, \\ \bar{u}_0(x-1) & 0 < x \le 1, \end{cases}$$

$$u_1(x) = \int_0^1 G(x,y)\delta(y-\alpha)dy = \begin{cases} (\alpha-1)x & 0 \le x < \alpha, \\ (x-1)\alpha & \alpha < x \le 1, \end{cases}$$

$$u_2(x) = -\int_0^1 G(x,y)\delta'(y-\alpha)dy = \begin{cases} -x & 0 \le x < \alpha, \\ 1-x & \alpha < x \le 1. \end{cases}$$

Adding the solutions,

$$u(x) = \int_0^1 G(x,y)\left\{-\bar{u}_0\delta'(y-0) + [u_x]\delta(y-\alpha) + \bar{u}_1\delta'(y-\alpha)\right\} dy,$$

and moving unknown terms to the left (with $[u_x] = -u_x^-$) results in (24). □

Remark 4.1 *The Schur-complement (22) shows how preconditioning (presumably $\mathcal{A}^{-1}$ can be applied in a fast manner) can also correspond to transforming a differential equation into an integral equation, here (24). The Schur-complement (23) shows how algebraic manipulations on the discrete system (applying $-D^T$) can correspond to transforming an integral formula into a boundary integral formula, here (25).*

Remark 4.2 *The biggest difference between the grid–aligned boundary case and the unaligned boundary case is the introduction of the new discrete variable C, an unknown jump. In higher dimensions, this means many jumps, their number "proportional" to the length of the boundary. However, using a fast solver for the regular problem and the Schur–complement (23), we see that we have discretized a Fredholm equation of the second kind on the boundary (25), which is well known to behave nicely numerically. This observation has borne out in numerical studies, see [10, 7] etc.*

Exercise 4.1. Find and prove an analogue of Lemma 1 for the case that (12) is replaced by $u_{xx} = f$ in (0,1).

4.4 Further examples of singular sources

In [8], Laplace's equations and the 2D linear elastic equations are solved quickly on the rectangle with various boundary conditions, by reflecting the solution in each dimension and solving periodic problems on the larger domains. There nonzero boundary conditions on the original rectangle enter as singular sources in the equation on the extended domains.

4.5 Comments on jump relations

One of the major steps of the EJIIM is the derivation of (one-sided) jump relations. We have seen that for Laplace's equation, $[u], [u_x]$ and the problem data $([f], [f_x], \dots)$ is all we need. In 2D, this is also true as was shown in [10] for the Laplace equation and in [9] for 2D linear elasticity. The idea in 2D is to take tangential derivatives on lower jumps and normal derivatives on the data, which we believe will extend to 3D without difficulties. In 3D, [6] have developed integral equations for just these jumps, based on the same ideas. The advantage of EJIIM over true boundary integral methods lies in its ability to deal with body forces and extendibility to variable coefficients; the drawback is that for problems where boundary integral methods apply, they are probably faster than EJIIM (for fixed quality of solution).

5 Conclusions

We have explained the relationship between a finite difference discretization of the Laplacian and Green's kernels. The usual discretization of Dirichlet boundary values at grid points was shown to be a special case of the EJIIM, and fast Poisson–solver based Schur–complements were shown to discretize integral formulas. These connections serve to explain the EJIIM also in higher dimensions, where some of the connections were made rigorous in [7].

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