Engineering Analysis with Boundary Elements 99 (2019) 23–28

Contents lists available at ScienceDirect

Engineering Analysis with Boundary Elements

journal homepage: www.elsevier.com/locate/enganabound

On the use of approximate fundamental solutions: Connections with the method of fundamental solutions and the method of regularized stokeslets

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ARTICLE INFO

Keywords:
Method of fundamental solutions
Method of regularized stokeslets
Laplace's equation
Stokes flow

ABSTRACT

Approximate fundamental solutions (AFS) are designed to be similar to fundamental solutions but without singularities. They have been used in the context of the Method of Fundamental Solutions and for problems of Stokes flow (where they are known as regularized stokeslets). A short survey of available AFS is given together with how they may be used to treat three-dimensional boundary-value problems for Laplace's equations. Explicit calculations are made for a sphere, with a focus on quantifying errors. It is concluded that the use of AFS can lead to unexpectedly large errors: caution is advised when abandoning true fundamental solutions.

1. Introduction

A fundamental solution for an elliptic partial differential equation (PDE) is a solution of the PDE with a singularity at one point. For Laplace's equation in three dimensions, the basic fundamental solution is

$$G_0(P,Q) = G_0(\boldsymbol{r};\boldsymbol{s}) = \mathcal{A}/R \quad \text{with} \quad R = |\boldsymbol{r}-\boldsymbol{s}|. \tag{1}$$

Here the points P and Q have position vectors $\boldsymbol{r}$ and $\boldsymbol{s}$, respectively, with respect to an origin O, and $\mathcal{A}$ is an arbitrary constant. Formally,

$$\nabla_Q^2 G_0(P,Q) = -4\pi\mathcal{A}\,\delta(\boldsymbol{r}-\boldsymbol{s}), \tag{2}$$

where $\delta(\boldsymbol{r})$ is the three-dimensional delta function. (This motivates the common choice $\mathcal{A} = -1/(4\pi)$.) Note that $G_0(P,Q) \sim \mathcal{A}/r$ as $r = |\boldsymbol{r}| \to \infty$ for fixed Q. Imposing this far-field condition renders G_0 unique.

We consider a model exterior boundary-value problem. It is to solve Laplace's equation, $\nabla^2 u = 0$, in B_e, the three-dimensional region exterior to a smooth closed bounded surface S. We impose a Dirichlet boundary condition, $u = f$ on S, where f is given. In addition, we require that $u(\boldsymbol{r}) = O(r^{-1})$ as $r \to \infty$. This problem is known to be uniquely solvable.

Classical potential theory reduces the boundary-value problem for u to a boundary integral equation over S. This reduction can be done in various ways; a brief review is given in Section 2. (See [1] for more information.) The resulting integral equations have kernels with singularities. Although these singularities can be handled without too much difficulty, many authors have been interested in developing methods without singularities. Two possibilities are as follows.

- Method of Fundamental Solutions (MFS). Here, $G_0(P, Q)$ is used but it is arranged that $P \neq Q$ by placing singularities inside S (see Section 3).
- Method of Approximate Fundamental Solutions (MAFS). Here, $G_0(P, Q)$ is replaced by $G_\eta(P, Q)$, containing a parameter η, chosen so that $G_\eta \to G_0$ as $\eta \to 0$ but $G_\eta(P, P)$ is finite when $\eta > 0$. Equivalently, the delta function on the right-hand side of Eq. (2) is replaced by a smooth 'blob function', $\phi_\eta(|\boldsymbol{r}-\boldsymbol{s}|)$, with $\phi_\eta(0)$ finite (see Section 4).

We are mainly concerned with the MAFS. Start with a standard integral representation for u, obtained by applying Green's theorem to u and G_0 in B_e,

$$4\pi\mathcal{A}\,u(P) = \int_S u(q)\frac{\partial G_0(P,q)}{\partial n_q}\,\mathrm{d}s_q - \int_S G_0(P,q)\frac{\partial u(q)}{\partial n}\,\mathrm{d}s_q, \quad P \in B_e, \tag{3}$$

where the unit normal vector on S points into B_e. The first term on the right-hand side is a double-layer potential. This term is known for our exterior Dirichlet problem because $u(q) = f(q)$, $q \in S$. The second term on the right is a single-layer potential. It is not known until we have computed $\partial u/\partial n$ on S, and this can be done in various ways (Section 2).

There is an integral representation similar to Eq. (3) for Stokes flow, with the analogues of u and $\partial u/\partial n$ being fluid velocity and force (traction) on S. The relevant fundamental solution is known as a *stokeslet* and then the corresponding MAFS is known as the *method of regularized stokeslets* [2].

If we replace G_0 by G_η in Eq. (3), we can expect good approximations to $u(P)$ when P is not near S, provided we know $u(q)$ and $\partial u/\partial n$ exactly. But this expectation may be thwarted if we try to compute these quantities using a method that itself uses G_η. Quoting from [3, p. 163]:

> It was demonstrated in [4] that the regularization error is $O(\eta^2)$ in the far field and only $O(\eta)$ in the near field, i.e. when the evaluation point is close to the boundary. This is true when the forces on the boundary are known to be exact. However, we have found that when

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https://doi.org/10.1016/j.enganabound.2018.11.001
Received 5 March 2018; Received in revised form 20 June 2018; Accepted 12 November 2018

the boundary force must be computed first from velocity boundary conditions, the error in the force turns out to be $O(\eta)$ because it comes from a near-field computation. This makes the error in all subsequent computations that use the force (even in the far field) to be $O(\eta)$.

Later, we shall confirm and quantify these observations using explicit analytical calculations for a sphere.

The paper quoted above [3] goes on to develop improvements but we claim that the basic approach is flawed: approximate fundamental solutions have their place (in vortex methods [5], for example) but their use negates a basic advantage of classical boundary integral methods and the MFS, namely, the exact satisfaction of both the governing PDE and the far-field condition.

2. Classical potential theory

There are two standard approaches, leading to a boundary integral equation for a certain quantity. One starts with an assumed integral representation for u (*indirect method*, Section 2.1) and the other starts from Green's theorem (*direct method*, Section 2.2). One strength of both approaches is that the PDE and the far-field condition are satisfied exactly, regardless of how well the relevant boundary quantity has been computed; errors in this computation imply errors in the satisfaction of the boundary condition.

2.1. Indirect method

Let us seek u in the form of a single-layer potential,

$$u(P) = \int_S \mu_0(q)\, G_0(P,q)\, \mathrm{d}s_q, \quad P \in B_\mathrm{e}, \tag{4}$$

where q denotes the integration point on S and $\mu_0(q)$ is to be found. This representation ensures that both $\nabla^2 u = 0$ and $u = O(r^{-1})$ as $r \to \infty$ are satisfied, for any continuous function μ_0. Applying the boundary condition gives

$$\int_S \mu_0(q)\, G_0(p,q)\, \mathrm{d}s_q = f(p), \quad p \in S, \tag{5}$$

a Fredholm integral equation of the first kind for μ_0.

One advantage of indirect methods is that, if μ_0 can be found, then we know that we have solved the boundary-value problem (which consists of the PDE, the boundary condition and the far-field condition). One disadvantage is that μ_0 does not usually have a physical interpretation. Note also that the starting point, namely Eq. (4), can be changed; for example, we could try writing $u(P)$ as a double-layer potential.

The kernel in Eq. (5), $G_0(p, q)$, has a weak singularity at $p = q$. The simplest way to handle this is to use a boundary element method. Thus partition S into N elements, $S = \cup_{j=1}^N S_j$. On S_j, approximate μ_0: $\mu_0(q) \simeq \mu_j^0$, a constant, when $q \in S_j$. Finally, evaluate Eq. (5) at $p = p_i$, $i = 1, 2, \ldots, N$, with $p_i \in S_i$. The result is the linear system

$$\sum_{j=1}^N \mu_j^0 \int_{S_j} G_0(p_i,q)\, \mathrm{d}s_q = f(p_i), \quad i = 1, 2, \ldots, N.$$

For $i \neq j$, we can use a simple approximation for the integrals (consistent with the simple piecewise-constant approximation for μ_0), giving

$$\sum_{\substack{j=1\\ j\neq i}}^N \mu_j^0 \big|S_j\big| G_0(p_i,p_j) + \mu_i^0 \int_{S_i} G_0(p_i,q)\, \mathrm{d}s_q = f(p_i), \quad i = 1, 2, \ldots, N, \tag{6}$$

where $|S_j|$ is the surface area of the boundary element S_j. The remaining integral has a weakly singular integrand and so has to be treated separately.

If we use the same approximations in Eq. (4), we obtain

$$u(P) \simeq \sum_{j=1}^N \mu_j^0 \int_{S_j} G_0(P,q)\, \mathrm{d}s_q \simeq \sum_{j=1}^N \mu_j^0 \big|S_j\big| G_0(P,p_j), \quad P \in B_\mathrm{e}. \tag{7}$$

This formula gives an approximate representation of $u(P)$ as a sum of point sources located on the boundary S. Evidently, this sum cannot be evaluated at $P = p_i$; it is also prone to numerical errors when P is close to S (although effective methods have been developed to resolve this difficulty).

2.2. Direct method

An application of Green's theorem to u and G_0 in B_e gives the integral representation for $u(P)$, Eq. (3). Letting $P \to p \in S$, taking into account the jump behaviour of the double-layer potential, and using the boundary condition gives

$$\int_S v(q)\, G_0(p,q)\, \mathrm{d}s_q = g(p), \quad p \in S, \tag{8}$$

a Fredholm integral equation of the first kind for $v = \partial u/\partial n$. In Eq. (8),

$$g(p) = -2\pi\mathcal{A}\, f(p) + \int_S f(q) \frac{\partial G_0(p,q)}{\partial n_q}\, \mathrm{d}s_q.$$

Using v, Eq. (3) becomes

$$u(P) = -\frac{1}{4\pi\mathcal{A}} \int_S v(q)\, G_0(P,q)\, \mathrm{d}s_q + F_0(P), \quad P \in B_\mathrm{e}, \tag{9}$$

where F_0 is computable from f,

$$F_0(P) = \frac{1}{4\pi\mathcal{A}} \int_S f(q) \frac{\partial G_0(P,q)}{\partial n_q}\, \mathrm{d}s_q. \tag{10}$$

Eqs. (8) and (9) can be discretized as in Section 2.1.

One advantage of direct methods is that the unknown function (here, it is v) has an immediate physical interpretation; indeed, it is often the desired quantity. One disadvantage is that we do not know if $u(P)$, defined by Eq. (9), actually satisfies the boundary condition (even though the boundary condition was used in order to derive Eq. (8)); showing this usually needs a separate argument [1, Section 5.6.5].

3. Method of fundamental solutions

The methods outlined in Section 2 lead to boundary integral equations with weakly-singular kernels. It is well known how to handle these singularities: effective efficient numerical methods have been developed [6].

Nevertheless some authors prefer to avoid computations involving singularities. One way is to use the so-called *method of fundamental solutions* (MFS). A continuous variant starts by modifying Eq. (4) to

$$u(P) = \int_{S_\gamma} v_\gamma(q)\, G_0(P,q)\, \mathrm{d}s_q, \quad P \in B_\mathrm{e}, \tag{11}$$

where v_γ is to be found and S_γ is similar to S but contained inside S. In more detail, suppose for simplicity that S is star-shaped with respect to the origin O; this means that every point $p \in S$ has position vector $\boldsymbol{r} = r(\theta,\phi)\hat{\boldsymbol{r}}$, where $\hat{\boldsymbol{r}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, θ and ϕ are spherical polar angles, and $r(\theta, \phi)$ is a single-valued function of those angles. Then points on S_γ have position vector $\boldsymbol{s} = (1-\gamma)r(\theta,\phi)\hat{\boldsymbol{r}}$ for sufficiently small $\gamma > 0$. Imposing the boundary condition on S gives

$$\int_{S_\gamma} v_\gamma(q)\, G_0(p,q)\, \mathrm{d}s_q = f(p), \quad p \in S. \tag{12}$$

This is an integral equation for v_γ; the kernel is non-singular because p and q lie on disjoint surfaces. We shall return to this method in Section 6.1.

A discrete (and much more popular) form of the MFS is as follows. Write

$$u(P) = \sum_{j=1}^N u_j G_0(P,q_j), \quad P \in B_\mathrm{e}, \tag{13}$$

where $q_j \in S_\gamma$. The coefficients u_j are determined by applying the boundary condition,

$$\sum_{j=1}^{N} u_j G_0(p_i, q_j) = f(p_i), \quad i = 1, 2, \ldots, N, \tag{14}$$

where $p_i \in S$. (The algebraic system may not be well conditioned, and so one may choose to impose the boundary condition at M points on S with $M > N$.)

For applications of the MFS to $\nabla^2 u = 0$ in three dimensions, see [7]. For analogous problems of Stokes flow, see [8,9].

4. Approximate fundamental solutions

Suppose that $\mathcal{G}(\rho)$ is defined for $\rho \geq 0$ as a smooth function with $\mathcal{G}(0) = \mathcal{B}$, $\mathcal{G}'(0) = 0$ and $\mathcal{G}(\rho) = \mathcal{A}/\rho + o(\rho^{-1})$ as $\rho \to \infty$, where $\mathcal{A}$ and $\mathcal{B}$ are arbitrary non-zero constants. Here $\mathcal{A}$, $\mathcal{B}$ and ρ are dimensionless.

Define G_η by

$$G_\eta(r) = \eta^{-1} \mathcal{G}(r/\eta), \tag{15}$$

where the quantity η is a length. Thus $G_\eta(0) = \mathcal{B}/\eta$,

$$G_\eta(r) = \mathcal{A}/r + o(r^{-1}) \quad \text{as } r \to \infty \text{ for fixed } \eta > 0, \tag{16}$$

and $G_\eta(r) = \mathcal{A}/r + o(1)$ as $\eta \to 0$ for fixed $r > 0$. These properties motivated calling G_η a *regularized fundamental solution*, regularized because $G_\eta(0)$ is finite. But G_η is not actually a fundamental solution because $\nabla^2 G_\eta(r) \neq 0$ for $r > 0$; *approximate fundamental solution* is a better terminology, as we shall see.

As G_η is spherically symmetric, we have

$$\nabla^2 G_\eta = G_\eta''(r) + (2/r) G_\eta'(r) = \eta^{-3} \left[\mathcal{G}''(r/\eta) + (2\eta/r) \mathcal{G}'(r/\eta) \right], \tag{17}$$

where the condition $\mathcal{G}'(0) = 0$ ensures that $\nabla^2 G_\eta$ is continuous at the origin. If we integrate $\nabla^2 G_\eta$ over a ball of radius r, B_r, Green's theorem gives

$$\int_{B_r} \nabla^2 G_\eta \, \mathrm{d}V = \int_{S_r} \frac{\partial G_\eta}{\partial r} \, \mathrm{d}s,$$

where S_r is the spherical boundary of B_r. Hence, assuming that $G_\eta'(r) \sim -\mathcal{A}/r^2$ as $r \to \infty$ (consistent with Eq. (16)),

$$\lim_{r \to \infty} \int_{B_r} \nabla^2 G_\eta \, \mathrm{d}V = -4\pi\mathcal{A}. \tag{18}$$

This result is necessary if we want to claim that $\nabla^2 G_\eta(r)$ is approximately a constant multiple of the three-dimensional Dirac delta function, $\delta(\boldsymbol{r})$. In addition, we want $\nabla^2 G_\eta$ to be localized, so that $\nabla^2 G_\eta(r) \to 0$ as $\eta \to 0$ for $r > 0$. Then we shall say that G_η is an *approximate fundamental solution*.

There are papers on approximations to $\delta(\boldsymbol{r})$; see [10] and references therein. However, we are interested in G_η rather than $\nabla^2 G_\eta$, and we shall require that G_η has the far-field behaviour given by Eq. (16) with $\mathcal{A} \neq 0$.

Rather than try to give general results, we consider a few examples. Perhaps the simplest is $\mathcal{G}(\rho) = \mathcal{A}(\rho^2 + 1)^{-1/2}$ leading to

$$\nabla^2 G_\eta = -\frac{3\mathcal{A}\eta^2}{(r^2 + \eta^2)^{5/2}} \quad \text{and} \quad G_\eta(r) = \frac{\mathcal{A}}{(r^2 + \eta^2)^{1/2}}. \tag{19}$$

To improve the decay of $\nabla^2 G_\eta$ as $\eta \to 0$, consider

$$\mathcal{G}(\rho) = \frac{\mathcal{A}(\rho^2 + c)}{(\rho^2 + 1)^{3/2}}, \tag{20}$$

where c is a constant. Then, using Eq. (17),

$$\nabla^2 G_\eta(r) = 3\mathcal{A}\eta^2 \left\{ (2c - 3) r^2 + (2 - 3c)\eta^2 \right\} (r^2 + \eta^2)^{-7/2}. \tag{21}$$

Setting $2c - 3 = 0$ gives the most rapid decay as $\eta \to 0$, leading to

$$\nabla^2 G_\eta = -\frac{15\mathcal{A}\eta^4}{2(r^2 + \eta^2)^{7/2}} \quad \text{and} \quad G_\eta(r) = \frac{\mathcal{A}(2r^2 + 3\eta^2)}{2(r^2 + \eta^2)^{3/2}}. \tag{22}$$

These formulas can be found in [11, Eqs. (6) and (15)]; see also [4, Eq. (9)] and [12, Eq. (4.1)]. We refer to the $\mathcal{G}$ defined by Eq. (20) as the *regularized fundamental solution*, since that terminology is commonly used. We shall use this $\mathcal{G}$ in Section 6.3 and a modified form of $\mathcal{G}$ in Section 6.4.

For another example, introduced by Beale [13, Eq. (2.19)], consider

$$\mathcal{G}(\rho) = \mathcal{A} \left\{ \rho^{-1} \operatorname{erf}(\rho) + c \, \mathrm{e}^{-\rho^2} \right\}, \tag{23}$$

where erf is the error function and c is a constant. Some calculation gives

$$\nabla^2 G_\eta(r) = \frac{2\mathcal{A}}{\eta^5} \left\{ 2cr^2 - \left(3c + \frac{2}{\sqrt{\pi}} \right) \eta^2 \right\} \mathrm{e}^{-r^2/\eta^2}.$$

The special case with $c = 0$ was used in [14, Eq. (3.7)]. Although not our concern here, it can be advantageous to choose c by imposing $\int_0^\infty r^4 \nabla^2 G_\eta(r) \, \mathrm{d}r = 0$. (Such moment conditions arise when analysing the approximation properties of approximate delta functions [4,10,12].) Imposing this moment condition yields $c = 1/\sqrt{\pi}$,

$$\nabla^2 G_\eta = \frac{2\mathcal{A}}{\eta^5 \sqrt{\pi}} \left(2r^2 - 5\eta^2 \right) \mathrm{e}^{-r^2/\eta^2} \quad \text{and} \quad G_\eta(r) = \mathcal{A} \left\{ \frac{\operatorname{erf}(r/\eta)}{r} + \frac{\mathrm{e}^{-r^2/\eta^2}}{\eta\sqrt{\pi}} \right\}. \tag{24}$$

The formula above for $\nabla^2 G_\eta$ can be found in [15] and in [12, Eq. (4.2)]. Beale [13, Eq. (2.19)] uses Eq. (23) with $c = 2/\sqrt{\pi}$; he imposes the moment condition $\int_0^\infty \{\rho\mathcal{G}(\rho) - \mathcal{A}\} \, \mathrm{d}\rho = 0$.

Further examples can be constructed using

$$\mathcal{G}(\rho) = \begin{cases} \mathcal{P}(\rho), & 0 \leq \rho < 1, \\ \mathcal{A}/\rho, & \rho > 1, \end{cases} \tag{25}$$

where $\mathcal{P}$ is a polynomial, leading to compactly supported formulas for $\nabla^2 G_\eta$. This is the main focus in [10]; see also [12, Eq. (4.3)]. The coefficients in $\mathcal{P}$ may be chosen so that G_η is differentiable at $r = \eta$. As an example, we have

$$\nabla^2 G_\eta = \begin{cases} \frac{15}{2} \mathcal{A} \eta^{-5} (r^2 - \eta^2), & 0 \leq r \leq \eta, \\ 0, & r \geq \eta, \end{cases} \tag{26}$$

$$G_\eta = \begin{cases} \frac{1}{8} \mathcal{A} \eta^{-5} (3r^4 - 10r^2\eta^2 + 15\eta^4), & 0 \leq r \leq \eta, \\ \mathcal{A}/r, & r \geq \eta. \end{cases} \tag{27}$$

The simplest example of the form in Eq. (25) has $\mathcal{P} = \mathcal{A}$, where the singularity is 'cut off'. The resulting *cut-off approximate fundamental solution* is harmonic for $r > 0$ but has a slope discontinuity at $r = \eta$. We shall return to this example in Section 6.2.

Another example (which can be written in the form of Eq. (25)) was suggested by Liu [16]:

$$G_\eta(r) = \frac{1}{|B_\eta|} \int_{B_\eta} G_0(\boldsymbol{r}, \boldsymbol{s}) \, \mathrm{d}V(\boldsymbol{s}), \tag{28}$$

where B_η is a ball of radius η with volume $|B_\eta| = \frac{4}{3}\pi\eta^3$. Some calculation shows that G_η is given by Eqs. (15) and (25) with $\mathcal{P}(\rho) = \frac{1}{2}\mathcal{A}(3 - \rho^2)$. Intuitively, this construction is attractive (smear fundamental solutions over a small ball) but $\nabla^2 G_\eta$ is discontinuous across $r = \eta$.

5. Use of approximate fundamental solutions

5.1. Direct method

Let $G_\eta(P, Q) = G_\eta(R)$ with $R = |\boldsymbol{r} - \boldsymbol{s}|$, the distance between P and Q. Then an application of Green's theorem to $u(Q)$ and $G_\eta(P, Q)$ in B_e gives

$$-\int_{B_e} u(Q)\,\nabla_Q^2 G_\eta(P,Q)\,\mathrm{d}V_Q = \int_S \left\{ u(q)\frac{\partial G_\eta(P,q)}{\partial n_q} - G_\eta(P,q)\frac{\partial u(q)}{\partial n}\right\}\mathrm{d}s_q, \quad P\in B_e. \tag{29}$$

This formula is [11, Eq. (9)]. It should be compared with Eq. (3).

The left-hand side of Eq. (29) can be written as

$$-u(P)\int_{B_e}\nabla_Q^2 G_\eta(P,Q)\,\mathrm{d}V_Q - \int_{B_e}[u(Q)-u(P)]\nabla_Q^2 G_\eta(P,Q)\,\mathrm{d}V_Q.$$

In this formula, the first integral is equal to

$$-4\pi\mathcal{A} - \int_{B_i}\nabla_Q^2 G(P,Q)\,\mathrm{d}V_Q = -4\pi\mathcal{A} - \int_S \frac{\partial G_\eta(P,q)}{\partial n_q}\,\mathrm{d}s_q,$$

where we have used Eq. (18) and B_i is the bounded domain enclosed by S. Thus, with $u = f$ and $v = \partial u/\partial n$ on S, Eq. (29) becomes

$$u(P) + E_\eta(P) = -\frac{1}{4\pi\mathcal{A}}\int_S v(q)\,G_\eta(P,q)\,\mathrm{d}s_q + F_\eta(P), \quad P\in B_e, \tag{30}$$

where

$$E_\eta(P) = \frac{u(P)}{4\pi\mathcal{A}}\int_S \frac{\partial G_\eta(P,q)}{\partial n_q}\,\mathrm{d}s_q - \frac{1}{4\pi\mathcal{A}}\int_{B_e}[u(Q)-u(P)]\nabla_Q^2 G_\eta(P,Q)\,\mathrm{d}V_Q, \tag{31}$$

$$F_\eta(P) = \frac{1}{4\pi\mathcal{A}}\int_S f(q)\frac{\partial G_\eta(P,q)}{\partial n_q}\,\mathrm{d}s_q. \tag{32}$$

Eq. (30) should be compared with Eq. (9). Both are exact. Unlike Eq. (9), the behaviour of Eq. (30) as $P\to p\in S$ is benign: there is no jump behaviour because G_η is not singular, so that we can simply replace P by p if we want to evaluate Eq. (30) on S.

The term F_η, Eq. (32), is expected and computable; see F_0 defined by Eq. (10). The term E_η, Eq. (31), is more troublesome. It may be called the *regularization error*. From Eq. (30), we obtain

$$f(p) + E_\eta(p) = -\frac{1}{4\pi\mathcal{A}}\int_S v(q)\,G_\eta(p,q)\,\mathrm{d}s_q + F_\eta(p), \quad p\in S. \tag{33}$$

This would be an integral equation for v if we knew $E_\eta(p)$: we do not, because it involves $u(Q)$ for all $Q\in B_e$. The usual practice is to discard E_η; see [4, Section III], [17] and [11, Section 2.1], where Eq. (22) is used. Some analyses of this approximation have been made [4,12] but these are not conclusive when P is on or near S; modifications have been proposed to handle these situations [11,12].

Suppose now that we have discarded E_η and then solved Eq. (33) (numerically), obtaining an approximation for $v(q)$. How should we then calculate $u(P)$? The answer is clear: we should abandon Eq. (30) and substitute our approximation for v into the standard integral representation Eq. (9) because that representation always generates a solution of $\nabla^2 u = 0$ regardless of the quality of the approximation to the true $v(q)$.

Beale [13] uses G_η in a different way. He starts with a standard direct boundary integral equation, derived using G_0. He then replaces G_0 by G_η, discretizes the integral equation (with a grid spacing h) and chooses η in terms of h. This leads to a provably convergent algorithm.

5.2. Indirect method

By analogy with the classical method sketched in Section 2.1, we could try writing

$$u(P) = \int_S \mu_\eta(q)\,G_\eta(P,q)\,\mathrm{d}s_q, \quad P\in B_e. \tag{34}$$

for some function μ_η; cf. Eq. (4). This formula incorporates the correct far-field behaviour for u but it does not ensure that $\nabla^2 u = 0$ everywhere in B_e. If P is sufficiently far from S, $G_\eta \simeq G_0$ and then $\nabla^2 u \simeq 0$ at such points P. This is true exactly if $\nabla^2 G_\eta$ is compactly supported (see Eq. (26), for example). Nevertheless, $\nabla^2 u = 0$ is not satisfied by Eq. (34) when P is close to S; this may be unfortunate because we have to impose the boundary condition on S. We shall study this point in Sections 6.2 and 6.3.

If we do apply the boundary condition to Eq. (34), we obtain

$$\int_S \mu_\eta(q)\,G_\eta(p,q)\,\mathrm{d}s_q = f(p), \quad p\in S. \tag{35}$$

Proceeding as in Section 2.1, we break S into N boundary elements and then approximate $\mu_\eta(q)$ by the constant μ_η^j on the jth element. The result is

$$\sum_{j=1}^N \mu_\eta^j \Big| S_j \Big| G_\eta(p_i,p_j) = f(p_i), \quad i = 1,2,\ldots,N. \tag{36}$$

This is simpler than Eq. (6) because $G_\eta(p_i,p_i)$ is finite. The numerical scheme described here and some variants have been used in [4,11,17].

Going further, we may propose a fully discrete version of the method (as was done with the method of fundamental solutions at the end of Section 3), writing

$$u(P) = \sum_{j=1}^N e_j G_\eta(P,p_j), \quad P\in B_e, \tag{37}$$

where the coefficients e_j are found by imposing the boundary condition,

$$\sum_{j=1}^N e_j G_\eta(p_i,p_j) = f(p_i), \quad i = 1,2,\ldots,N. \tag{38}$$

Numerical experiments based on this approach have been reported [16,18].

6. Explicit calculations when S is a sphere

When S is a sphere, explicit analytical calculations can be made, thus permitting clearer assessments of the various methods described above. We consider the simplest possible problem, a sphere of radius a with boundary condition $u = 1$ on $r = a$. The exact solution is $u = a/r$.

6.1. Continuous version of the MFS

The MFS was described in Section 3, where the continuous variant is based on the integral representation Eq. (11), a distribution of sources over the surface S_γ, which we take as a concentric sphere of radius $b < a$. The spherical symmetry of the problem implies that the source density v_γ is a constant. In order to integrate over S_γ, use spherical polar coordinates so that the point P is on the z-axis at $z = r$. Then the integration with respect to the azimuthal angle gives a factor of 2π. Hence, making use of Eq. (1), Eq. (11) reduces to

$$u(r) = 2\pi v_\gamma\mathcal{A}\int_0^\pi \frac{b^2\sin\vartheta\,\mathrm{d}\vartheta}{\sqrt{r^2+b^2-2br\cos\vartheta}}, \quad r > a.$$

The integration is elementary:

$$u(r) = 2\pi v_\gamma\mathcal{A}b^2\left[\frac{\sqrt{r^2+b^2-2br\cos\vartheta}}{br}\right]_0^\pi = \frac{C}{r},$$

where the constant $C = 4\pi v_\gamma\mathcal{A}b^2$. Application of the boundary condition gives $C = a$.

It is not surprising that the exact solution is recovered. First, the integral representation Eq. (11) generates exact solutions of Laplace's equation, with no singularities outside the sphere $r = b$. Second, the exact solution of the boundary-value problem, $u = a/r$ can be continued analytically inside the boundary, $r = a$: no singularities are encountered between $r = a$ and $r = b$. There is a singularity at $r = 0$, but it is inside $r = b$.

6.2. MAFS with a cut-off $\mathcal{G}$

Consider the cut-off approximate fundamental solution, defined by

$$\mathcal{G}(\rho) = \begin{cases} \mathcal{A}, & 0 \le \rho < 1, \\ \mathcal{A}/\rho, & \rho \ge 1. \end{cases} \tag{39}$$

Proceeding as in Section 6.1, starting from Eqs. (34) and (15), we arrive at

$$u(r) = 2\pi a^2 \frac{\mu_\eta}{\eta} \int_0^\pi \mathcal{G}\Big(\eta^{-1}\sqrt{r^2+a^2-2ar\cos\vartheta}\,\Big) \sin\vartheta \,\mathrm{d}\vartheta, \quad r > a,$$

where μ_η is a constant. Evaluation depends on the value of r/a: when r/a is sufficiently large, the cut-off is not needed (so that $\rho > 1$ in Eq. (39)) whereas the cut-off is needed when r/a is close to 1. Specifically, there are two regions, an outer region in which $r > a+\eta$, and an inner region in which $a < r < a+\eta$.

In the outer region, $\rho > 1$, so that

$$u(r) = 2\pi a^2 \frac{\mu_\eta}{\eta} \int_0^\pi \frac{\mathcal{A}\eta \sin\vartheta \,\mathrm{d}\vartheta}{\sqrt{r^2+a^2-2ar\cos\vartheta}} = \frac{C}{r}, \quad r > a+\eta, \tag{40}$$

where $C = 4\pi\mu_\eta \mathcal{A} a^2$ is a constant. The fact that $u(r)$ is proportional to $1/r$ when $r > a+\eta$ is expected; this is the only non-constant spherically symmetric solution of Laplace's equation.

In the inner region, $a < r < a+\eta$, we can define an angle ϑ_0 corresponding to

$$\rho = \eta^{-1}\sqrt{r^2+a^2-2ar\cos\vartheta_0} = 1,$$

and then

$$\begin{aligned} u(r) &= 2\pi a^2 \frac{\mu_\eta}{\eta} \int_{\vartheta_0}^\pi \frac{\mathcal{A}\eta \sin\vartheta \,\mathrm{d}\vartheta}{\sqrt{r^2+a^2-2ar\cos\vartheta}} + 2\pi a^2 \frac{\mu_\eta}{\eta} \int_0^{\vartheta_0} \mathcal{A}\sin\vartheta \,\mathrm{d}\vartheta \\ &= \frac{C}{4ar\eta}\big\{2\eta(r+a-\eta) + \eta^2 - (r-a)^2\big\}, \quad a < r < a+\eta. \end{aligned} \tag{41}$$

This formula contains a piece proportional to r, namely $-Cr/(4a\eta)$, so that $\nabla^2 u \neq 0$ in the inner region. Nevertheless, applying the boundary condition, $u = 1$ at $r = a$, determines C,

$$C = 4a^2/(4a-\eta) = a(1-\varepsilon/4)^{-1} \quad \text{with} \quad \varepsilon = \eta/a$$

(assuming that $\varepsilon \neq 4$). This can be substituted in Eq. (40) to give u in the outer region. As the exact solution is $u_{\mathrm{ex}} = a/r$, the relative error is

$$\frac{u-u_{\mathrm{ex}}}{u_{\mathrm{ex}}} = \Big(1-\frac{\varepsilon}{4}\Big)^{-1} - 1 = O(\varepsilon) \quad \text{as } \varepsilon \to 0.$$

This error is uniform in r, assuming that $r > a(1+\varepsilon)$.

In the inner region, we can put $r = a(1+\delta)$ where $0 < \delta < \varepsilon$. Then Eq. (41) gives

$$\frac{u-u_{\mathrm{ex}}}{u_{\mathrm{ex}}} = \Big(1-\frac{\varepsilon}{4}\Big)^{-1}\Big(1-\frac{(\varepsilon-\delta)^2}{4\varepsilon}\Big) - 1 \sim \frac{\delta}{4\varepsilon}(2\varepsilon-\delta) \quad \text{as } \varepsilon \to 0.$$

Of course, there is no error at the boundary ($\delta = 0$) but otherwise the relative error is seen to be $O(\varepsilon)$. We note that $u(r)$ and $u'(r)$ are continuous across $r = a+\eta$.

6.3. MAFS with the regularized $\mathcal{G}$

Consider the regularized $\mathcal{G}$ defined by Eq. (20) as

$$\mathcal{G}(\rho) = \frac{\mathcal{A}(\rho^2+c)}{(\rho^2+1)^{3/2}} = \frac{\mathcal{A}}{(\rho^2+1)^{1/2}} + \frac{\mathcal{A}(c-1)}{(\rho^2+1)^{3/2}}, \tag{42}$$

where c is a constant (often taken as $c = \frac{3}{2}$; see text below Eq. (21)). Using Eqs. (34) and (15), together with $\rho = \eta^{-1}\sqrt{r^2+a^2-2ar\cos\vartheta}$, we obtain

$$u(r) = \frac{C}{2}\int_0^\pi \left(\frac{1}{(\mathcal{R}^2-2ar\cos\vartheta)^{1/2}} + \frac{\eta^2(c-1)}{(\mathcal{R}^2-2ar\cos\vartheta)^{3/2}}\right)\sin\vartheta\,\mathrm{d}\vartheta,$$

where $\mathcal{R}^2 = r^2+a^2+\eta^2$ and $C = 4\pi\mu_\eta\mathcal{A}a^2$ (as before). Evaluating the integral,

$$\begin{aligned} u(r) = \frac{C}{2ar}\big[&(\mathcal{R}^2+2ar)^{1/2} - (\mathcal{R}^2-2ar)^{1/2} \\ &- \eta^2(c-1)\big\{(\mathcal{R}^2+2ar)^{-1/2} - (\mathcal{R}^2-2ar)^{-1/2}\big\}\big]. \end{aligned} \tag{43}$$

The quantity in square brackets can be expanded in powers of a/r; we find that

$$u(r) = \frac{C}{r}\left(1 + \frac{\varepsilon^2}{2}(2c-3)\frac{a^2}{r^2} + O((a/r)^4)\right) \quad \text{as } r \to \infty, \tag{44}$$

thus verifying that the error can be minimized by taking $2c-3 = 0$.

Applying the boundary condition, $u(a) = 1$, to Eq. (43) gives

$$\begin{aligned} 1 &= \frac{C}{2a}\left[\sqrt{4+\varepsilon^2} - \frac{\varepsilon^2(c-1)}{\sqrt{4+\varepsilon^2}} + \varepsilon(c-2)\right] \\ &= \frac{C}{a}\left(1 + \frac{\varepsilon}{2}(c-2) - \frac{\varepsilon^2}{8}(2c-3) + O(\varepsilon^4)\right) \quad \text{as } \varepsilon \to 0. \end{aligned} \tag{45}$$

When this result is combined with Eq. (44), we see that the relative error is $O(\varepsilon)$, even in the far field, and even with the special choice $c = \frac{3}{2}$. Indeed, it appears that the choice $c = 2$ gives a smaller relative error at a cost of an erroneous contribution of $O((a/r)^2)$ to the far field.

In the near field, put $r = a(1+\delta)$. Then, with $\delta = O(\varepsilon)$, Eq. (43) gives

$$u(r) \simeq \frac{C}{r}\left(1 + \frac{\delta}{2} + \frac{1}{2\sqrt{\varepsilon^2+\delta^2}}\big((c-2)\varepsilon^2 - \delta^2\big)\right). \tag{46}$$

When combined with Eq. (45), we again see first-order relative error:

$$\frac{u-u_{\mathrm{ex}}}{u_{\mathrm{ex}}} \simeq \frac{1}{2\sqrt{\varepsilon^2+\delta^2}}\left\{\delta\Big(\sqrt{\varepsilon^2+\delta^2}-\delta\Big) - \varepsilon(c-2)\Big(\sqrt{\varepsilon^2+\delta^2}-\varepsilon\Big)\right\}.$$

6.4. MAFS with another regularized $\mathcal{G}$

Let us introduce another free parameter c' into the regularized $\mathcal{G}$ of Section 6.3, and define

$$\mathcal{G}_3(\rho) = \mathcal{G}(\rho) + c'\mathcal{A}(\rho^2+1)^{-5/2} \tag{47}$$

where $\mathcal{G}$ is defined by Eq. (42). Proceeding as in Section 6.3, we add a term

$$\frac{C}{2}\int_0^\pi \frac{\eta^4 c' \sin\vartheta\,\mathrm{d}\vartheta}{(\mathcal{R}^2-2ar\cos\vartheta)^{5/2}} = \frac{C\eta^4 c'}{6ar}\big\{(\mathcal{R}^2-2ar)^{-3/2} - (\mathcal{R}^2+2ar)^{-3/2}\big\}$$

to the right-hand side of Eq. (43). This has no effect on the far-field estimate in Eq. (44) but it changes Eq. (45) into

$$1 = \frac{C}{a}\left(1 + \frac{\varepsilon}{6}(3c+c'-6) - \frac{\varepsilon^2}{8}(2c-3) + O(\varepsilon^4)\right) \quad \text{as } \varepsilon \to 0.$$

Thus the choices $c = c' = \frac{3}{2}$ give $C/a = 1 + O(\varepsilon^4)$ as $\varepsilon \to 0$ and then Eq. (44) gives $(u-u_{\mathrm{ex}})/u_{\mathrm{ex}} = O((a/r)^4)$ as $r \to \infty$. In the near field, a term $\frac{1}{6}(C/r)c'\varepsilon^4(\varepsilon^2+\delta^2)^{-3/2}$ is added to the right-hand side of Eq. (46): the near-field relative error remains as first order, for any choices of c and c' in $\mathcal{G}_3$.

7. Comparisons, comments and conclusions

Let us write Eq. (37) as

$$u(\boldsymbol{r}) = \sum_{j=1}^N e_j G_\eta(|\boldsymbol{r}-\boldsymbol{r}_j|).$$

This is one starting point for the use of radial basis functions (RBFs) to solve boundary-value problems [19]. However, in those methods, the nodes at $\boldsymbol{r}_j$ lie on S and in B_{e}, and then $\nabla^2 u = 0$ is imposed at points $\boldsymbol{r}$ in B_{e}. Here, all the nodes are on the boundary, and the boundary condition

is imposed at those nodes; the task of satisfying $\nabla^2 u = 0$ is delegated to the choice of G_η. This connection with RBF methods was noted by Gáspár [18, p. 373].

It is interesting to compare the discrete forms of the MFS and the MAFS for the simplest problem, a sphere of radius a. For the MFS, with collocation points p_i at $\boldsymbol{r}_i$ and source points q_j at $\boldsymbol{s}_j$, we have

$$\begin{aligned}|\boldsymbol{r}_i - \boldsymbol{s}_j|^2 &= |\boldsymbol{r}_i|^2 + |\boldsymbol{s}_j|^2 - 2\boldsymbol{r}_i \cdot \boldsymbol{s}_j \\ &= a^2 + (1-\gamma)^2 a^2 - 2a^2(1-\gamma)\hat{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{r}}_j \\ &= (1-\gamma)a^2\big\{2(1 - \hat{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{r}}_j) + \gamma^2/(1-\gamma)\big\}.\end{aligned}$$

The entries in the system matrix Eq. (14) are proportional to $|\boldsymbol{r}_i - \boldsymbol{s}_j|^{-1}$.

For the MAFS, we require $G_\eta(R)$, where

$$R^2 = |\boldsymbol{r}_i - \boldsymbol{r}_j|^2 = 2a^2(1 - \hat{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{r}}_j).$$

As before, write $\eta = \varepsilon a$, with ε positive and dimensionless. Then, using the simplest approximate fundamental solution, Eq. (19),

$$G_\eta(p_i, p_j) = \frac{\mathcal{A}}{\sqrt{R^2 + \eta^2}} = \frac{\mathcal{A}}{a\sqrt{2(1 - \hat{\boldsymbol{r}}_i \cdot \hat{\boldsymbol{r}}_j) + \varepsilon^2}}.$$

We see that, for this special case, the MFS and the MAFS lead to exactly the same linear system when $\eta = \gamma a/\sqrt{1-\gamma}$. We note that the MAFS can be refined by using other choices for G_η (Section 4) but the MFS always generates an exact solution of the governing PDE.

We conclude that gains in simplicity stemming from the use of approximate fundamental solutions can be outweighed by doubts concerning lack of accuracy and lack of rigour.

Acknowledgments

I thank the referees for their constructive comments including the suggestion to make the calculations in Section 6.4.

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