Applicability of the method of fundamental solutions

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Abstract

The condition number of a matrix is commonly used for investigating the stability of solutions to linear algebraic systems. Recent meshless techniques for solving partial differential equations have been known to give rise to ill-conditioned matrices, yet are still able to produce results that are close to machine accuracy. In this work, we consider the method of fundamental solutions (MFS), which is known to solve, with extremely high accuracy, certain partial differential equations, namely those for which a fundamental solution is known. To investigate the applicability of the MFS, either when the boundary is not analytic or when the boundary data is not harmonic, we examine the relationship between its accuracy and the effective condition number.

Three numerical examples are presented in which various boundary value problems for the Laplace equation are solved. We show that the *effective condition number*, which estimates system stability with the right-hand side vector taken into account, is roughly inversely proportional to the maximum error in the numerical approximation. Unlike the proven theories in literature, we focus on cases when the boundary and the data are not analytic. The effective condition number numerically provides an estimate of the quality of the MFS solution without any knowledge of the exact solution and allows the user to decide whether the MFS is, in fact, an appropriate method for a given problem, or what is the appropriate formulation of the given problem.

Key words: Laplace equation, Method of Fundamental Solutions, Effective condition number, Error estimation

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1 Introduction

The method of fundamental solutions (MFS) introduced by Kupradze and Aleksidze [23] has become a popular meshless method for solving various partial differential equations (PDEs) of practical importance; for example, Poisson equations [13], nonlinear Poisson problems [2], nonlinear thermal explosions [5], diffusion-convection equations [26], acoustic scattering [21], elastic waves [22] and inverse problems [15,31]. See [10,11,14] for comprehensive reviews of applications of the MFS. The method falls in the class of methods called boundary methods. Like the boundary element method (BEM), it is applicable when a fundamental solution of the differential equation in question is known, and it shares the same advantages as the BEM over domain discretization methods. Moreover, it has certain advantages over the BEM. In the MFS, the user simply provides the location of the boundary of the domain of the problem. There is no need to create a mesh over the entire region or its boundary. Since meshing can quickly turn into a time consuming task depending on the complexity of the region, this aspect of the MFS can save considerable computational time. Moreover, since the MFS is a boundary-type meshless method, it is also computationally much cheaper than other domain-type meshless methods; see [24] for an overview. More importantly, the accuracy of some MFS approximations can approach the order of machine epsilon. This last benefit may seem somewhat paradoxical since the linear systems arising in this method are ill-conditioned. Our interest, on the other hand, is to investigate when such high order accuracy is likely to occur.

A brief outline of the remainder of this paper is as follows. In Section 2, we provide a short overview of the formulation and implementation of the MFS for the solution of the Laplace equation. Some MFS convergence theories will also be reviewed in Section 3. In Section 4, we discuss the conditioning of a matrix and formally introduce the condition number and effective condition number. We examine the use of the effective condition number $\kappa_{\text{eff}}(A, b)$ as an estimator of the MFS accuracy, and observe a relationship between the effective condition number and the accuracy of the MFS solution. From the results of various numerical experiments, it appears that the accuracy is inversely proportional to the *effective condition number* κ_{eff}, that is,

$$\kappa_{\text{eff}}(A, b) = \mathcal{O}\left({\varepsilon_{\max}}^{-1}\right) \quad \text{where } \varepsilon_{\max} = \sup_{P \in \Omega} |u_N(P) - u(P)|. \tag{1}$$

Here, $\varepsilon_{\max}$ is a measure of the maximum error of the numerical solution over the region of interest. Section 5 contains three numerical examples which exhibit the relationship (1). Finally, in Section 6, we summarize our results and form a conclusion, as well as suggest new paths of future research.

2 Formulations

For experimental purposes, we examine the solution of the Laplace equation

$$\triangle u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{in } \Omega \subset \mathbb{R}^2, \tag{2}$$

where Ω is either the unit disk $\bigcirc$ or the square $\square = [-1, 1]^2$. The boundary of Ω, $\partial\Omega$, is divided into two boundary segments, Γ_0 and Γ_1, such that $\partial\Omega = \Gamma_0 \cup \Gamma_1$ and $\Gamma_0 \cap \Gamma_1 = \emptyset$. The boundary conditions that we consider are either of the Dirichlet-type or the mixed-type. Specifically, the Dirichlet boundary conditions are given by the function g_0, and the Neumann boundary conditions are given by the function g_1 such that

$$u = g_0 \quad \text{on } \Gamma_0, \qquad \frac{\partial u}{\partial n} = g_1 \quad \text{on } \Gamma_1. \tag{3}$$

For problems with Dirichlet boundary conditions only, we simply set $\Gamma_1 = \emptyset$. The solution to (2) is therefore of the form of $u(\cdot\,; g_0, g_1, \Omega)$.

By a fundamental solution of the Laplace equation we mean a function $K(P, Q)$ such that

$$\Delta K(P, Q) = -\delta(P, Q), \quad P, Q \in \mathbb{R}^n, \;\; n = 2, 3,$$

where $\delta(P, Q)$ ($\int \delta \, d\mathbb{R}^2 = 1$ if $P = Q$ or otherwise 0) denotes the Dirac delta function. It is well known that

$$K(P, Q) = -\frac{1}{2\pi} \log \|P - Q\|,$$

which is defined everywhere except when $P = Q$, where it is singular. Thus Q is called a singularity, or *source point*. In the MFS, the solution of the PDE is represented by a linear combination of fundamental solutions, so that, in the case of the Laplace equation in $\mathbb{R}^2$, we set

$$u_N(P) = a_0 + \sum_{j=1}^{N} a_j \log \|P - Q_j\| \quad \text{for } P \in \overline{\Omega}, \tag{4}$$

where $\|\cdot\|$ is the Euclidean norm in $\mathbb{R}^2$. In the present work, a_0 will be set to zero.

The source points $\{Q_j\}_{j=1}^N \subset \partial\tilde{\Omega}$ are preassigned on the boundary of a fictitious domain and located outside the domain of the problem. Consequently, u_N satisfies the Laplace equation in Ω, which implies that the MFS is a Trefftz method. The unknown coefficients $\{a_j\}_{j=1}^N$ in (4) are determined so that u_N collocates the boundary conditions at certain specified points. Specifically,

we let $\{P_k\}_{k=1}^N$ be $N = N_0 + N_1$ collocation points on $\partial\Omega$ ordered in such a way that the first N_0 points are on Γ_0 and are associated with the Dirichlet boundary conditions in (3), while the remaining $N - N_0$ are on Γ_1 and are associated with the Neumann boundary conditions. Then the coefficients $\{a_j\}_{j=1}^N$ are chosen to exactly satisfy

$$\begin{aligned} u_N(P_k) &= g_0(P_k), \quad P_k \in \Gamma_0, & 1 \le k \le N_0, \\ \frac{\partial}{\partial n} u_N(P_k) &= g_1(P_k), \quad P_k \in \Gamma_1, & N_0 + 1 \le k \le N. \end{aligned}$$

Using (4), we obtain an $N \times N$ system of linear equations,

$$\begin{aligned} \sum_{j=1}^{N} a_j \log \|P_k - Q_j\| &= g_0(P_k), & 1 \le k \le N_0, \\ \sum_{j=1}^{N} a_j \frac{\partial}{\partial n} \log \|P_k - Q_j\| &= g_1(P_k), & N_0 + 1 \le k \le N, \end{aligned}$$

that can be solved using various methods. In all of the numerical experiments reported in this paper, we employ the *MATLAB*'s backslash function for convenience.

3 Convergence Theories of the MFS

Assume that Ω and the fictitious domain $\tilde{\Omega}$ are concentric circles of radius r and R, respectively. We may also assume that the circles are centered at the origin,

$$\Omega = \{x : \|x\|_2 < r\}, \quad \tilde{\Omega} = \{x : \|x\|_2 < R\}.$$

For Laplace equations with Dirichlet boundary condition, that is, $\Gamma_1 = \emptyset$ in (3), let the collocation points $\{P_k\}_{k=1}^N$ and source points $\{Q_j\}_{j=1}^N$ be uniformly distributed on $\partial\Omega$ and $\partial\tilde{\Omega}$, respectively. In [17,19] it is shown that if u is harmonic in the entire plane, then

$$\varepsilon_{\max} = \mathcal{O}\left(\left(\frac{r}{R}\right)^N\right).$$

This result is generalized in [20] to the case that the harmonic extension of u exists only in a larger but bounded disk. If we only assume g_0 to be analytic, then $\varepsilon_{\max} = \mathcal{O}(\tau^N)$ for some $\tau < 1$. In [18], the MFS exponential convergence theory is generalized to regions in the plane whose boundaries are analytic Jordan curves.

The overview above gives us the motivation of the presented work, but it is not our aim to study the convergence theories of the MFS here. We end this

short section with the following remark: *there is no convergence theory for the MFS applied to non-harmonic Dirichlet boundary $\partial\Omega$ with non-harmonic boundary data g_0.*

4 The Conditioning of Matrix Systems

The condition number and the concept of conditioning were introduced by Turing [30]. The condition number of a nonsingular square matrix A is defined by $\kappa = \kappa(A) = \|A\|\|A^{-1}\|$. In the case where the matrix 2-norm is used, the condition number can be expressed as $\kappa(A) = \sigma_1/\sigma_n$, where σ_1 and σ_n are the largest and smallest singular values of A, respectively. Note that $\kappa \geq 1$. The matrix A is said to be *well-conditioned* if $\kappa \approx 1$, and *ill-conditioned* if $\kappa \gg 1$. Given some small perturbation, Δb, of the right-hand side vector b, the condition number estimates the stability of the solution. Specifically, if $Ax = b$ and $A(x + \Delta x) = b + \Delta b$, then

$$\frac{\|\Delta x\|}{\|x\|} \leq \kappa \frac{\|\Delta b\|}{\|b\|}. \tag{5}$$

One result of this is that one can expect to lose $\log_{10} \kappa$ decimal digits when solving the system in floating point arithmetic [29].

In [7,17], it is shown that the 2-norm (original) condition number κ of the MFS matrix grows exponentially with N,

$$\kappa = \mathcal{O}\left(\log R^{N/2} \left(\frac{R}{r}\right)^{N/2}\right). \tag{6}$$

Although the problem of ill-conditioning of the MFS is widely reported in the literature, the accuracy of the numerical solution is rarely affected [6] *when u is harmonic on the entire plane.* All numerical examples in this paper are dealing with the MFS matrix system with condition number $\kappa(A) > 10^{18}$.

In many applications, the boundary may not be analytic. Furthermore, if boundary data are only analytic but not harmonic, then we do not know how far the harmonic extension of u may extend. In some cases, the boundary data may contain noise. Clearly, we can no longer rely solely on the condition number to predict the accuracy of the computed solution of all practical ill-conditioned MFS systems. Most importantly, the accuracy of the MFS has an obvious dependence on the right-hand vector.

Since the condition number does not involve the right-hand side vector b, any examination of the stability of the system only considers the worst case scenario no matter the choice of b. In many applications, b is problem-dependent

but fixed. In this case, we are interested in the stability of the system with this specific problem-dependent b, and are not concerned with the worst case scenario. For these reasons, as a tool to estimate of the accuracy of the MFS, we consider the effective condition number $\kappa_{\text{eff}} = \kappa_{\text{eff}}(A, b)$, which is defined in the following way.

Consider a full-rank matrix $A \in \mathbb{R}^{M\times N}$, $M \geq N$, with singular values $\sigma_1 \geq \ldots \geq \sigma_N > 0$. and the SVD decomposition $A = U\Sigma V^*$ where $U \in \mathbb{R}^{M\times M}$ and $V \in \mathbb{R}^{N\times N}$ contains the singular vectors, $\Sigma = \text{Diag}(\sigma_1, \ldots, \sigma_N) \in \mathbb{R}^{M\times N}$. Denotes $U = [u_1, \ldots, u_M]$ and $V = [v_1, \ldots, v_N]$, respectively, by their columns. Consider a perturbed matrix system $A(x + \Delta x) = b + \Delta b$. We can write

$$b = \sum_{i=1}^{M} \beta_i u_i, \quad \Delta b = \sum_{i=1}^{M} \Delta\beta_i u_i$$

and let $\beta = (b_1, \ldots, b_N)^T = U^* b$ and $\Delta\beta = (\Delta b_1, \ldots, \Delta b_N)^T = U^*\Delta b$. The least-squares solution can be expressed in terms of the pesudoinverse of A, namely

$$x = A^\dagger b := V\Sigma^\dagger U^T b, \quad \Delta x = A^\dagger \Delta b.$$

Suppose $p \leq N$ is the largest integer such that $\sigma_p > 0$. Then

$$\Sigma^\dagger = \text{Diag}(\sigma_1^{-1}, \ldots, \sigma_p^{-1}, \underbrace{0, \ldots, 0}_{N-p}) \in \mathbb{R}^{N\times M}.$$

Since U is orthogonal, we have

$$\|x\| = \sqrt{\sum_{i=1}^{N} \left(\frac{\beta_i}{\sigma_i}\right)^2}, \quad \|\Delta x\| = \sqrt{\sum_{i=1}^{N} \left(\frac{\Delta\beta_i}{\sigma_i}\right)^2} \leq \frac{\|\Delta b\|}{\sigma_N}.$$

Putting these to the inequality (5) results in a new bound with κ replaced by the *effective condition number* for $Ax = b$ given by

$$\kappa_{\text{eff}}(A, b) = \|b\| \Big/ \sigma_N \sqrt{\left(\frac{\beta_1}{\sigma_1}\right)^2 + \ldots + \left(\frac{\beta_N}{\sigma_N}\right)^2}.$$

In case of $M = N$, the pseudoinverses will simply become the standard matrix inverses; all claims remain valid.

The effective condition number was introduced and studied in Chan and Foulser [4]. Subsequently, it was applied to boundary element methods in Christiansen and Hansen [8] and Christiansen and Saranen [9].

The effective condition number determines the conditioning of a linear system with coefficient matrix A and a fixed vector b. Like the condition number, if the effective condition number is small, then a small perturbation Δb of the vector b will result in a small change in x. If the effective condition number is

large, a small perturbation Δb made to the fixed b will result in large changes in x. Note that $\kappa_{\text{eff}}(A, b) \leq \kappa(A)$ for all choices of b, and equality is achieved when $b = u_1$ is the first left singular vector or any vector in that direction.

Other kinds of effective condition numbers are given in Banoczi et al. [3], where they are applied to Gaussian elimination and the QR factorization. More recent references for the effective condition number can be found in [16,25].

In the next section, under different settings, to some of which the MFS convergence theories do not applied, we present some numerical evidence to show that the effective condition number κ_{eff} is a good indicator of the accuracy of the MFS. What we want to observe is that whenever the MFS results in high accuracy, the κ_{eff} will be large (e.g. same magnitude as the inverse of machine epsilon). At the same time, when the MFS results in poor accuracy, the κ_{eff} will be moderate in size too.

5 Numerical Experiments

Our goal is to demonstrate the strong linkage between the effective condition number κ_{eff} and the accuracy $\varepsilon_{\max}$ of the MFS in order to support our conjecture (1). As a preliminary study, (i) we will only consider square matrix systems. For the ease of reproducing our results, we keep the set up of the MFS straightforward. We are not claiming that the overdetermined formulation is of less importance: if noise in data is detected (say, by small κ_{eff} in Example 5.1), it is very natural to solve the system with the least-squares fitting. The trivial way to obtain the $N \times N$ MFS matrix systems is to impose equal numbers of collocation points and source points, as in Section 3. Hence, (ii) we do not append any constant in the numerical expansion (4). Because of that, the source points will not be placed on the unit circle to avoid the origin being null.

In the following three examples, several parameters known to affect the accuracy of MFS approximations are varied. In each example, the relationship between the accuracy of the approximation and the effective condition number is examined. In the first example, Section 5.1, noise is added to the boundary data. The presence of noise causes small changes in b while keeping the matrix A unchanged. Section 5.2 further examines the relationship for problems with harmonic and non-harmonic boundary data on both analytic boundary $\Omega = \bigcirc = \{x : \|x\|_2 < 1\}$ and non-analytic boundary $\Omega = \square = \{x : \|x\|_\infty < 1\}$. Finally, in Section 5.3, compatible and incompatible mixed boundary conditions on the boundary of the square $\square$ are considered.

The positioning of the points on the boundary and the source points outside the region is a much discussed topic. For all the examples in this paper, it is sufficient to use 160 boundary data points equally spaced along the boundary of the region. An equal number of source points is used. Each corresponds to a boundary collocation point and is located a distance R along the outward normal to the boundary at that boundary point; the fictitious domain, containing the region of interest, is given by

$$\tilde{\Omega} = \{x \in \mathbb{R} \setminus \Omega : \inf_{y \in \Omega} \|x - y\| < R\}. \tag{7}$$

By the maximum principle, if u is a continuous real-valued harmonic function defined in a bounded region Ω, then u attains its maximum and minimum values on the boundary $\partial\Omega$; see [1]. Thus the maximum error will always occur on the boundary since $u_N(x) - u(x; g_0, g_1, \Omega)$ is harmonic. We determine the accuracy of the solution by finding the maximum absolute error on the boundary $\partial\Omega$ re-defined by

$$\varepsilon_{\max} = \max_{x \in X_{\text{test}}} |u_N(x) - u(x; g_0, g_1, \Omega)|, \tag{8}$$

where $X_{\text{test}} \subset \partial\Omega$ is a set of 640 boundary test points.

5.1 Noise Tolerance

In this example, the Laplace equation is solved in the unit disk ◯ subject to the Dirichlet boundary condition prescribed by the harmonic function

$$f_0(x, y) = e^x \cos y.$$

Additive noise, generated by *Matlab*© 's `RAND` function, is then systematically added to the boundary data. The matrix A is solely determined by the positioning of the boundary collocation points and the source points, while the right-hand side vector is determined by the boundary data $g_0 = f_0$ and the imposed noise level. Thus, the noise will only affect the right-hand side vector b but not the MFS matrix. The condition number of the system will remain constant 2.35×10^{19} while the effective condition number and accuracy will change as noise is added.

It is well known that the MFS is very susceptible to noisy boundary data. For the noise free case, we expect the MFS to produce results extremely close to machine accuracy since u is harmonic in $\mathbb{R}^2$. As the percentage of noise added to the vector b is increased, we see in Table 1 that the effective condition number decreases and maximum absolute error increases. We observed a

Table 1
$f_0(x, y) = e^x \cos y$ on circular boundary with source distance $R = 2.0$

Noise Percent	κ_{eff}	$\varepsilon_{\max}$
0.000%	2.84×10^{15}	2.36×10^{-14}
0.005%	1.45×10^{6}	6.06×10^{-4}
0.050%	8.34×10^{4}	1.38×10^{-2}
0.100%	3.27×10^{4}	5.34×10^{-2}
0.500%	3.59×10^{3}	1.14×10^{-1}
1.000%	2.32×10^{3}	1.16×10^{-1}

sharp increase in error and an equally sharp decrease in the effective condition number as a tiny amount of noise is added.

Going from noise-free to noisy data, the effective condition number drops from 2.84×10^{15} with no noise to 1.45×10^{6} with just 0.005% noise suggesting again that the numerical solution is very sensitive to perturbation to b. Hence, when only 0.005% of noise is added in, the MFS accuracy drops by 10 orders of magnitude. The estimated perturbation by κ_{eff}, from (5), is

$$\|\Delta x\|_\infty \leq 0.005\% \kappa_{\text{eff}} \|x\|_\infty = 0.005\% (2.84 \times 10^{15})(2.718) = 3.86 \times 10^{11}.$$

The uncertainty principle of Schaback [28] to radial basis function interpolation problems seems to hold here too. What we see here is that: *for the MFS, there is a conflict between theoretically achievable accuracy and numerical stability measured by the* effective condition numbers.

Even though all runs in Table 1 have exactly the same condition number, completely different error behaviors are observed in cases with higher noise levels. The resulting effective condition numbers and maximum errors are very similar for test cases with 0.500% and 1.000% noise; that suggests those systems are not too sensitive to the added noise

The data in Table 1 strongly support the relation (1). As more noise is added, the relationship becomes weaker, but by this point the effective condition number is small enough ($\kappa_{\text{eff}} \approx 10^4$) to indicate that the MFS solution will not be of machine epsilon accuracy. This example is a good starting point to show the relationship between the accuracy of the MFS and effective condition number because only the right-hand vector b is altered. All else stays4 constant, including the ill-conditioned matrix A.

5.2 Boundary Shapes

In this example, we examine the effect of changing the source distance R in (7) with different boundary data on different domains. The Laplace equation with the Dirichlet boundary condition on both $\bigcirc$ and $\square$ is tested. Two Dirichlet boundary conditions are considered, a constant (harmonic) function,

$$c_0(x, y) = 1, \quad (x, y) \in \partial\Omega,$$

and a non-harmonic polynomial,

$$q_0(x, y) = x^2 y^3, \quad (x, y) \in \partial\Omega.$$

A caution of setting up MFS numerical examples is brought up by Schaback [27]: one will always obtain excellent results *independent of the boundary shape* when the boundary conditions generated by an exact *harmonic* solution (e.g., $g_0 = u|_{\Gamma_0}$ and $\nabla u = 0$ in $\mathbb{R}^2$). Poor results are achieved only when the boundary data are generated from a non-harmonic function so that u does not have a harmonic extension in $\mathbb{R}^2$.

When the boundary data are generated from the harmonic function c_0, by the theories in Section 3, *on both domains*, we expect to see the MFS achieving high accuracy. In Figure 1, it is clear that the MFS solutions $u(\cdot\,; c_0, -, \bigcirc)$ and $u(\cdot\,; c_0, -, \square)$ almost always achieve the best results no matter the source distance or boundary shape. The harmonic boundary data from c_0, which in the majority of situations allow the MFS to achieve high accuracy on both boundary shapes, also produce the highest effective condition number ($\kappa_{\text{eff}} \approx 10^{16}$); see Figure 2 and Table 2.

For the non-harmonic polynomial q_0, note in Figure 2, the effective condition numbers for q_0 on $\bigcirc$ are much higher than that on $\square$ for all tested R. These results agree well (inversely) with the behavior of the corresponding MFS accuracy; see Table 3 for details. Unlike the case of harmonic data, the accuracy associated with q_0 does depend on R. Since the solutions to non-harmonic boundary function on $\bigcirc$ are much more likely to have a harmonic extension beyond the domain [12], the accuracy of the MFS solution $u(\cdot\,; q_0, -, \bigcirc)$ should converge exponentially in theory and is numerically much better than $u(\cdot\,; q_0, -, \square)$. But the accuracy of $u(\cdot\,; q_0, -, \bigcirc)$ decreases as the source distance increases; with analytic boundary and analytic data, this seems to contradict the theories in Section 3 that the accuracy should increase with larger R. All condition numbers in this example are reported to be around 10^{21} by *Matlab*© 's `COND` function but they are not trustworthy. Using (6), we are sure that the condition number increases with R which is the main reason of the

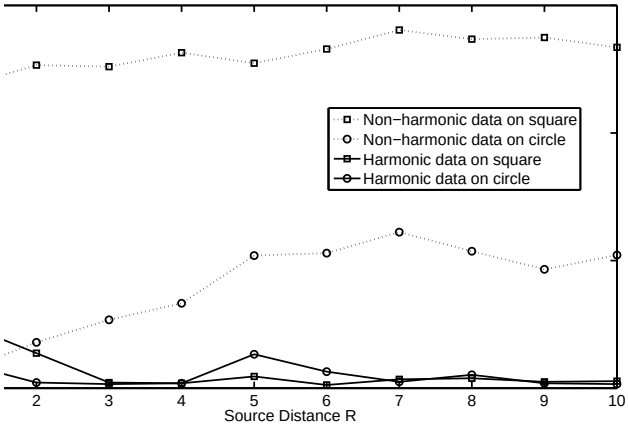

Fig. 1. Accuracy of MFS approximations for different boundary data on square and circle.

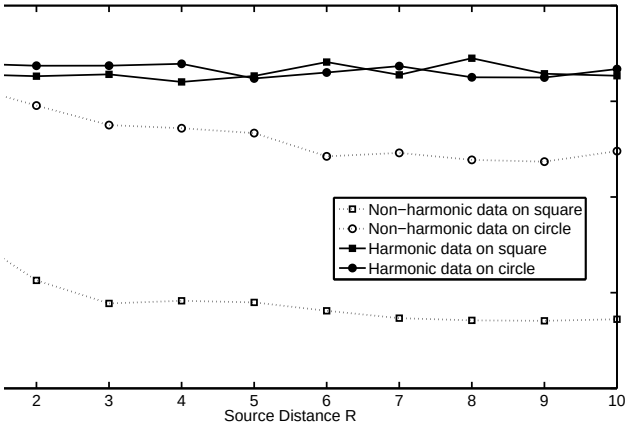

Fig. 2. Effective condition numbers of MFS linear systems for different boundary data on square and circle.

drop in accuracy. Previous literatures also show that this theory does not necessarily hold in practical computations. Drop in accuracy when R increases is also observed in [6]. The important observation here is that *the* κ_{eff} *in fact decreases with* R *to reflect such losses in accuracy.*

5.3 Mixed Boundary Conditions

Our final example examines the Laplace equation with compatible and incompatible mixed boundary conditions on the square domain $\square$. For the incompatible case, the imposed Dirichlet and Neumann conditions are inconsistent. Here, Γ_1, a connected subset of $\partial\Omega$ with length $|\Gamma_1| = 2$, begins from certain angles θ; see Figure 3 for a demonstration. We let Γ_1 rotate around the boundary with different starting θ to generate different test problems. We use

	Square		Circle	
Source radius R	$\varepsilon_{\max}$	κ_{eff}	$\varepsilon_{\max}$	κ_{eff}
1	3.3185e-013	2.6169e+016	9.2149e-015	9.4692e+016
2	2.3537e-014	2.0330e+016	1.6653e-015	7.1766e+016
3	1.6653e-015	2.5508e+016	1.4433e-015	7.2547e+016
4	1.5543e-015	1.0190e+016	1.5543e-015	8.9926e+016
5	2.8866e-015	2.0981e+016	2.1316e-014	1.5503e+016
6	1.3323e-015	1.1144e+017	4.4409e-015	3.1772e+016
7	2.2204e-015	2.4001e+016	1.7764e-015	6.8918e+016
8	2.4425e-015	1.7688e+017	3.3307e-015	1.7927e+016
9	1.7764e-015	2.7224e+016	1.5543e-015	1.7349e+016
10	1.8874e-015	2.1567e+016	1.4433e-015	4.7970e+016

Table 2
Errors and effective condition numbers as functions of R for Harmonic data on square and circle

	Square		Circle	
Source radius R	$\varepsilon_{\max}$	κ_{eff}	$\varepsilon_{\max}$	κ_{eff}
1	6.5586e-004	1.3358e+008	4.9336e-015	6.8663e+015
2	4.5747e-003	4.3713e+005	6.2280e-014	5.9494e+014
3	3.9648e-003	2.7303e+004	4.7556e-013	5.6837e+013
4	1.4041e-002	3.7725e+004	2.1221e-012	3.9095e+013
5	5.4202e-003	3.0807e+004	1.5775e-010	2.1678e+013
6	1.9512e-002	1.1286e+004	1.9574e-010	1.3202e+012
7	1.0813e-001	4.6614e+003	1.3021e-009	2.0046e+012
8	4.7500e-002	3.5699e+003	2.3262e-010	8.6361e+011
9	5.4887e-002	3.3896e+003	4.5293e-011	6.9648e+011
10	2.2810e-002	4.0727e+003	1.6498e-010	2.4736e+012

Table 3
Errors and effective condition numbers as functions of R for non-harmonic data on square and circle

the harmonic functions $c_0 = 1$ and $f_0 = e^x \cos y$ as g_0 in (2) to generate the Dirichlet boundary conditions, while the Neumann boundary conditions on Γ_1 are set to zero, that is, $g_1 = 0$ in (3).

Since the numbers of source points and collocation points are equal, we have

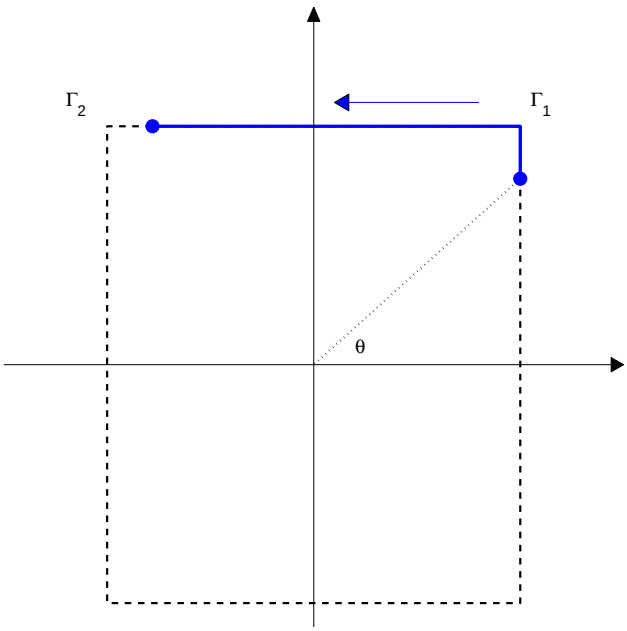

Fig. 3. Schematic setup for problem 5.3

an exactly determined system and the numerical approximation exactly satisfies the collocation conditions. This can lead to higher accuracy than an overdetermined system that uses a best fitting for approximation. However, this method is not without its own challenges. An exactly determined system can lead to the estimation greatly over shooting or under shooting the actual boundary values in between the data points. This phenomenon is known as the Gibbs effect. For this example, the maximum absolute error along the boundary can no longer be measured since we no longer have a complete set of Dirichlet boundary values for (8). The maximum norm, $\|\cdot\|_\infty$, of the numerical solution is used as a measure here.

The maximum norm of the solution is used to detect the magnitude of the Gibbs effect in the solution and thus give an indicator as to whether or not the solution may be accurate. However, it is important to note that the maximum norm does not indicate the maximum absolute error of a solution. This means that two solutions may have the similar maximum norm but much different maximum absolute error. It should also be noted by the reader that the maximum norm only indicates that the solution *may* be accurate and not the maximum error–*we use the effective condition number to detect bad solutions* in this example.

Figure 4 shows the expected small norm for the constant case in c_0. The exact solution $u(\cdot\,; 1, 0, \square)$ is the constant-1 function. Since the function $c_0 = 1$ is harmonic everywhere, we expect to see very good accuracy and thus its maximum norm will stay at 1. Figure 5 shows the effective condition number.

The *Shift* on the x-axis of the plot indicates the starting angle θ for Γ_1. Since the solution to c_0 is harmonic, the consistently good results are accompanied by the consistently high effective condition numbers ($\kappa_{\text{eff}} \approx 10^{16}$).

In the case of f_0, we do not except any good result from our exactly determined approach, since

$$\frac{\partial f_0}{\partial n} \neq 0 \quad \text{for all } (x, y) \in \partial\square, \tag{9}$$

the boundary data are not compatible for all θ. As seen in Figure 4, the MFS solutions have very large norm of certain θ values indicating the presence of the Gibbs effect. Good results are still possible, but only if a harmonic extension of u exists beyond $\partial\Omega$ for some particular θ-positions of Γ_1.

To justify the relation (1), note that the norms of solutions behave with respect to the effective condition number and reach relative minima at $\pi/4$, $3\pi/4$, $5\pi/4$, and $7\pi/4$. This leads us to believe that there is a harmonic extension for these problem settings. It is important for the reader to note that, although the maximum norm can be used as an indicator for good accuracy, it cannot show exactly how accurate the solution is. It is for this reason that the vast differences between the effective condition numbers of the two functions are not as pronounced in Figure 4.

The results when using f_0 are very interesting. The effective condition number starts off relatively small, but then increases and has a relative maximum around $\pi/4$. It then decreases to close to its original value and has another relative maximum $\pi/2$ radians later. The pattern, *small* κ_{eff} *associated with large* $\|u_N\|_\infty$ *(e.g. Gibbs)*, repeats periodically. From a geometric perspective, the effective condition number achieves a relative maximum whenever Γ_1 is positioned totally on one side of the square boundary. Combining the numerical intuition and observed κ_{eff} values, we may guess that u has a harmonic extension beyond $\square$ when the incompatible boundary conditions are connected at the singularities of the $\partial\Omega$.

Before ending this section, we emphasize again that square systems are used here because they are trivial to set up and easy to reproduce. The effective condition numbers are used as an indicator for data quality but not for solving the problem. In this example, when a small effective condition number is observed and the Gibbs effect is present, the user should impose extra collocation points and conditions in order to extend the existing square system to an overdetermined one.

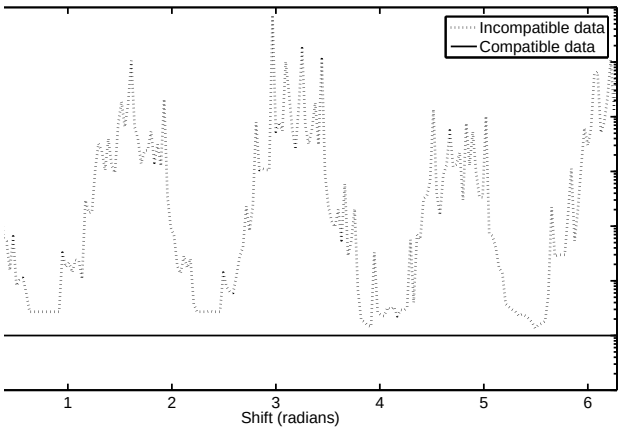

Fig. 4. Norm of the MFS solution for compatible and incompatible boundary data on square.

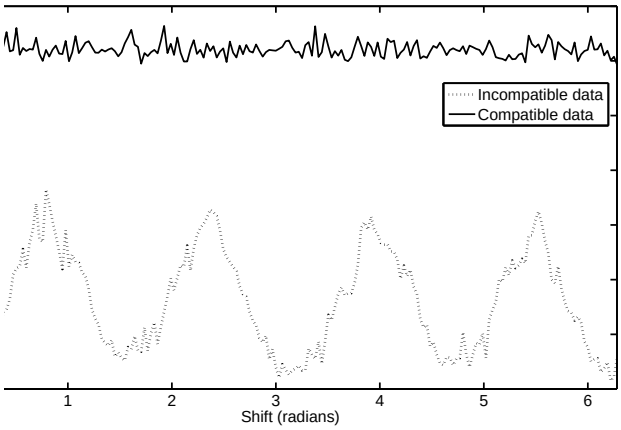

Fig. 5. Effective condition numbers of MFS resultant systems for compatible and incompatible boundary data on square.

6 Conclusion

In summary, we have presented numerical evidence that there is a strong relationship between the effective condition number of a linear system and the accuracy of results when using the method of fundamental solutions, namely *high MFS accuracy must accompany a large "effective" condition number*. In order to obtain machine accuracy, from the presented numerical results, the effective condition number of the MFS systems should stay around 10^{16}. In the future, other elliptic operators along with the overdetermined formulation should be examined to ensure the validity of this uncertainty principle. This not only includes additional systems generated by the MFS, but also ill-conditioned systems arising in other methods that still achieve good results for specific right-hand side vectors. In addition, there is much theoretical investigation that needs done in this area of numerical analysis.

While further investigation is needed, some applications can already be envisioned. One can use the effective condition number to determine if the MFS is a feasible method for solving the partial differential equation in hand. The attraction of the MFS is the high accuracy that it is able to obtain. However, as shown in the presented numerical examples, the high accuracy of the MFS cannot be guaranteed under all situations. The effective condition number of the linear system generated by the MFS can help determine whether or not the MFS is a practicable method, or if overdetermination, regularization, etc. are needed in the formulation.

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