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Effective Condition Number for Boundary Knot Method

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Abstract: This study makes the first attempt to apply the effective condition number (ECN) to the stability analysis of the boundary knot method (BKM). We find that the ECN is a superior criterion over the traditional condition number. The main difference between ECN and the traditional condition numbers is in that the ECN takes into account the right hand side vector to estimates system stability. Numerical results show that the ECN is roughly inversely proportional to the numerical accuracy. Meanwhile, using the effective condition number as an indicator, one can fine-tune the user-defined parameters (without the knowledge of exact solution) to ensure high numerical accuracy from the BKM.

Keywords: boundary knot method, effective condition number, traditional condition number.

1 Introduction

In recent years, a variety of boundary meshless methods have been introduced, such as the method of fundamental solutions (MFS)[Fairweather and Karageorghis (1998);Young, Tsai, Lin, and Chen (2006);Chen, Karageorghis, and Smyrlis (2008)], boundary knot method (BKM) [Chen and Tanaka (2002);Chen and Hon (2003);Wang, Chen, and Jiang (2009)], boundary collocation method [Chen, Chang, Chen, and Lin (2002);Chen, Chen, Chen, and Yeh (2004)], boundary node method [Mukherjee and Mukherjee (1997);Zhang, Yao, and Li (2002)], and regularized meshless method [Young, Chen, and Lee (2005);Young, Chen, Chen, and Kao (2007);Chen, Kao, and Chen (2009)]. All these methods are of the boundary type numerical technique in which only the boundary knots are required in the numerical solution of homogeneous problems.

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Despite the evident merits of the MFS being integration-free, super-convergent, and easy-to-use [Golberg and Chen (1998);Li (2001);Qin, Wang, and Kompis (2009)], the method also has perplexing drawbacks in requiring fictitious boundary outside the physical domain. The artificial boundary is somewhat arbitrary and not trivial to determine without prior knowledge of problems of interest, which causes the method less applicable to practical engineering problems with complicated boundary geometry and multiply-connected domains.

To overcome the above-mentioned problems in the MFS, Chen and coworkers [Chen and Tanaka (2002)] recently introduced the boundary knot method, which uses the non-singular trial functions such as T-complete functions [Kita, Kamiya, and Ikeda (1995)] or general solutions instead of the singular fundamental solution in the MFS. Thus, the collocation and observation points can coincident and be placed on the physical boundary of the problem in the BKM.

It is noted that both the MFS and the BKM are of a global interpolation approach enjoying high convergence rate. On the other hand, their full interpolation matrix tends to be severely ill-conditioned when using a large number of boundary knots. Consequently, small perturbations, e.g., measurement or computer rounding errors, in boundary data may result in an enormous divergence in the final solution.

The L^2 condition number has been used to measure the conditioning of the interpolation matrix of the MFS and the BKM. Contradicting to the conventional wisdom. It is observed in many reports that even if the L^2 condition number is extensively huge when using a large number of knots, the resulting numerical accuracy, however, is surprisingly high [**Liu (2008a);Liu and Atluri (2009);Liu, Yeih, and Atluri (2009);**Wang, Chen, and Jiang (2009)]. In some cases, we can get accurate solution while the L^2 condition number analysis indicates that numerical solutions of the BKM or the MFS are not reliable. This means that the L^2 condition number negatively overestimates these global interpolation methods.

It is well known that the resulting discretization algebraic equation of the MFS and the BKM can be expressed in the standard form $Ax = b$. The effective condition number is introduced to replace the L^2 condition number in the estimation of conditioning of the global interpolation methods [Chan and Foulser (1988);Christiansen and Hansen (1994);Li and Huang (2008a);Li and Huang (2008b)]. Their difference lies in that the former considers the effect of the right hand side vector b. In particular, reference [Drombosky, Meyer, and Ling (2009)] proposes a new effective condition number to more accurately measure the conditioning of the MFS interpolation.

In this study, we extend the use of the effective condition number to the BKM. Similar to the case of MFS, we find that numerical accuracy of the BKM is also inversely proportional to the corresponding effective condition number, that is to say, ECN $= \mathcal{O}(\varepsilon_{max}^{-1})$, where ε_{max} is the maximum error in computational domain. The ECN can also be effectively used to determine the optimal knot number with the boundary knot method without any knowledge on the (unknown) exact solution.

This paper is organized as follows. In Section 2, the formulation of BKM is reviewed. Section 3 introduces the effective condition number, followed by Section 4 to present numerical experiments and discussions. We conclude this paper with some remarks in section 5.

2 BKM formulation

Without loss of generality, we consider the Helmholtz boundary value problem stated as follows:

$$\nabla^2 u + \lambda^2 u = 0 \quad \text{in} \quad \Omega \tag{1}$$

$$u(x) = \bar{u}(x) \quad \text{on} \quad \Gamma_D \tag{2}$$

$$q(x) = \frac{\partial u}{\partial n} = \bar{q}(x) \quad \text{on} \quad \Gamma_N \tag{3}$$

where $\bar{u}(x)$ and $\bar{q}(x)$ are known functions, Ω denotes the solution domain in $\Re^d$ with boundary $\partial\Omega = \Gamma_D \cup \Gamma_N$ where d represents the dimensionality of the space and n the unit outward normal.

In the case λ is purely imaginary, we have the modified Helmholtz equation:

$$\nabla^2 u - \lambda^2 u = 0 \quad \text{in } \Omega. \tag{4}$$

The non-singular general solutions of the homogeneous Helmholtz equation(1) and homogeneous modified Helmholtz equation (4) are, respectively, given by

$$u_n^*(r) = \left(\frac{\lambda}{2\pi r}\right)^{(n/2)-1} J_{(n/2)-1}(\lambda r), \ \ n \geq 2, \tag{5}$$

and

$$u_n^*(r) = \frac{1}{2\pi}\left(\frac{\lambda}{2\pi r}\right)^{(n/2)-1} I_{(n/2)-1}(\lambda r), \ \ n \geq 2, \tag{6}$$

where J represents the Bessel function of the first kind, I denotes the modified Bessel functions of the first kind, and r means the Euclidean norm distance. In the BKM, all collocation knots are placed only on physical boundary and can be used either as source or response points which cures the major problem of fictitious boundary facing the MFS.

By using the non-singular general solution(5) or (6) as the trial basis function, the numerical solution of Eq. (1) can be represented by

$$u(x) = \sum_{j=1}^{N} \alpha_j u_n^*(\|x - \xi_j\|) \tag{7}$$

where j is the index of source points on physical boundary, N denotes the total number of boundary knots $\{\xi_1, \xi_2, \ldots, \xi_N\} \subset \partial\Omega$ and α_j $(j = 1, \ldots, N)$ are the unknown expansion coefficients. By collocating boundary equations (2) and (3) at all collocation knots $\{x_1, x_2, \ldots, x_N\} \subset \partial\Omega$, we have N equations given as

$$\sum_{k=1}^{N} \alpha_k u_n^*(r_{ik}) = \bar{u}(x_i), \quad x_i \in \Gamma_D \tag{8}$$

$$\sum_{k=1}^{N} \alpha_k \frac{\partial u_n^*(r_{jk})}{\partial n} = \bar{q}(x_j), \quad x_j \in \Gamma_N. \tag{9}$$

Note that for any small wave number λ, $\nabla^2 u \pm \lambda^2 u = 0$, the so-called quasi-Laplace equation, is a good approximation to the Laplace equation. Either non-singular general solution (5) or (6), with sufficiently small λ, can be used to solve $\nabla^2 u = 0$. Eqs. (8) and (9) can be written in the following $N \times N$ matrix system

$$A\alpha = b, \tag{10}$$

where $A = (A_{ij})$ is an interpolation matrix and $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)^T$. We notice that being a global interpolation approach, the BKM produces a highly ill-conditioned and dense coefficient matrix, in particular when using a large number of boundary knots, which is clearly reflected by its associated huge L^2 condition number [Wang, Chen, and Jiang (2009)]. **For such ill-conditioned systems encountered in dealing with delay ordinary differential equations or nonlinear partial differential equations, Liu et al [Liu and Atluri (2008);Liu (2008b);Liu (2009)] proposed a fictitious time integration method.**

It is worthy noting that the L^2 condition number measures the conditioning of interpolation matrix by a ratio of the maximum and minimum singular values of the interpolation matrix A. This is the worst case scenario among all possible right hand vectors. The *fixed* vector b in the right hand side of Eq. (10) is usually not the worst case in the L^2 condition number. As an alternative measurement index, the effective condition number is introduced to include the effect of the vector b [Drombosky, Meyer, and Ling (2009)]. More details are given in the next section.

3 Measurement of interpolation matrix conditioning

The L^2 condition number of a nonsingular square matrix A in Eq. (10) is defined by $\text{Cond}(A) = \parallel A \parallel \cdot \parallel A^{-1} \parallel$, where the matrix 2−norm is used, the L^2 condition number can be stated as $\text{Cond}(A) = \sigma_1/\sigma_n$, σ_1 and σ_n are the largest and smallest singular value of A, respectively.

As a matter of fact, the matrix A can be decomposed by singular value decomposition as

$$A = UDV^T, \tag{11}$$

where $U = [u_1, u_2, \cdots, u_N]$ and $V = [v_1, v_2, \cdots, v_N]$ are orthogonal matrices, $U^T U = V^T V = I_N$, where I_N denotes the identity matrix and D is a diagonal matrix with diagonal elements

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N \geq 0, \tag{12}$$

where $\sigma_i, 1 \leq i \leq N$ are called the singular values of A while the vectors u_i and v_i are the left and right singular vectors of A, respectively.

Substituting Eq.(11) into Eq.(10), we have

$$\alpha = \sum_{i=1}^{N} \frac{u_i^T b}{\sigma_i} v_i. \tag{13}$$

In some cases, the boundary data b may be disturbed by some noise. Clearly, we should not rely solely on the L^2 condition number to predict the accuracy of the computed solution of all practical ill-conditioned BKM systems. Most importantly, the accuracy of the BKM has an obvious dependence on the right hand vector. Since the L^2 condition number does not involve the right hand side vector b, any research of the stability of the system regardless of the choice of b is not appropriate. 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 among all possible right hand vectors. Under these conditions, as a tool to estimate the accuracy of the BKM, we consider the effective condition number $\text{ECN} = \text{ECN}(A, b)$, which is defined as follows [Drombosky, Meyer, and Ling (2009)].

Consider a perturbed matrix system $A(x + \triangle x) = b + \triangle b$. We can derive

$$b = \sum_{i=1}^{N} \beta_i u_i, \quad \triangle b = \sum_{i=1}^{N} \triangle \beta_i u_i. \tag{14}$$

Let $\beta = (b_1, ..., b_N)^T = U^* b$ and $\triangle\beta = (\triangle b_1, ..., \triangle b_N)^T = U^* \triangle b$. The solution can be expressed in terms of the inverse of A, namely

$$x = A^{-1}b := VD^{-1}U^T b, \quad \triangle x = A^{-1}\triangle b. \tag{15}$$

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

$$D^{-1} = \mathrm{Diag}(\sigma_1^{-1}, ..., \sigma_p^{-1}, 0, ..., 0). \tag{16}$$

Since U is orthogonal, we have

$$\| x \| = \sqrt{\sum_{i=1}^{N} (\frac{\beta_i}{\sigma_i})^2}, \quad \| \triangle x \| = \sqrt{\sum_{i=1}^{N} (\frac{\triangle\beta_i}{\sigma_i})^2} \leq \frac{\| \triangle b \|}{\sigma_N}. \tag{17}$$

If $Ax = b$ and $A(x + \triangle x) = b + \triangle b$, then

$$\frac{\| \Delta x \|}{\| x \|} \leq \mathrm{Cond}(A) \frac{\| \Delta b \|}{\| b \|} \tag{18}$$

Substituting Eq.(17) into the inequality(18) results in a new error bound for Eq.(10) with ECN, as an alternative replacement of L^2 condition number

$$\mathrm{ECN}(A, b) = \frac{\| b \|}{\sigma_N \sqrt{\left(\frac{\beta_1}{\sigma_1}\right)^2 + ... + \left(\frac{\beta_N}{\sigma_N}\right)^2}}. \tag{19}$$

Section 4 will investigate the relationship between solution accuracy and the effective condition number.

4 Numerical results and discussions

To demonstrate the relationship between the ECN of a linear system and its accuracy of results when using the boundary knot method, several numerical results are considered for homogeneous Helmholtz and modified Helmholtz problems. To verify the claim under the influence of noise, random number is added to the discrete boundary conditions by

$$u = \overline{u} + \delta, \quad q = \overline{q} + \delta, \tag{20}$$

where $\overline{u}, \overline{q}$ are the exact boundary values, respectively, in (2) and (3). We use the uniform random number generator to produce random numbers Rand in $[-1, 1]$ and let $\delta = \varepsilon \times \mathrm{Rand}$ where ε denotes the level of the noise.

4.1 Case 1: Helmholtz equation with noisy data

In this case, the homogeneous Helmholtz equation (1) with an elliptic domain $\Omega = \{(x,y) : x^2/4 + y^2 = 1\}$ with only Dirichlet boundary is considered. Wave number is taken to be $\lambda = \sqrt{2}$ with corresponding analytical solution given by $u = \sin(x)\cos(x)$. The matrix A is solely determined by the positioning of the boundary knots, while the right hand side vector is determined only by Dirichlet boundary data and the imposed noise level. Thus, the added noise will only affect the right hand side vector b but not the BKM coefficient matrix.

Table 1: Elliptic domain for case 1: Number of boundary knot is $N = 30$, and number of randomly distributed boundary test knots is $M = 150$.

Noise percent	Cond	ECN	ε_{max}
0.0	2.74×10^{17}	4.87×10^{9}	5.37×10^{-8}
0.001	2.74×10^{17}	1.37×10^{5}	7.49×10^{-4}
0.005	2.74×10^{17}	2.04×10^{4}	5.60×10^{-3}
0.01	2.74×10^{17}	1.53×10^{4}	9.20×10^{-3}
0.05	2.74×10^{17}	1.76×10^{3}	6.40×10^{-2}
0.1	2.74×10^{17}	1.40×10^{3}	7.07×10^{-2}
0.5	2.74×10^{17}	1.94×10^{2}	5.67×10^{-1}

It is seen from Table 1 that the ECN decreases while the maximum absolute error increases. We observe a shape drop in the effective condition number as a tiny amount of noise is added. 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 data in Table 1 strongly support the relation $\text{ECN} = \mathcal{O}(\varepsilon_{max}^{-1})$. As more noise is added, the relationship becomes weaker, but by this point the effective condition number is small enough $(\text{ECN} \leq 10^3)$ to indicate that the BKM solution will not be accurate enough. This example is a proper starting point to show the relationship between the accuracy of the BKM and the effective condition number because only the right hand vector b is altered with all other factors, including the ill-conditioned matrix A, stay constant.

4.2 Case 2: modified Helmholtz equation with noisy data

Similar to Case 1, the homogeneous modified Helmholtz equation (4) on a unit square domain $\Omega = \{(x,y)|0 < x < 1, 0 < y < 1\}$ is solved under the influence of noise. Two Dirichlet boundary $x = 1$ and $y = 1$ and others Neumann boundary is considered. Accompanied with analytical solution $u = e^{(x+y)}$, λ in the corresponding non-singular general solution (6) is equal to $\sqrt{2}$. Number of boundary knot is $N = 116$, and $M = 900$ domain test knots are randomly chosen over the region of interest.

Table 2: A unit square domain with mixed boundary conditions for case 2.

Noise percent	Cond	ECN	ε_{max}
0.0	1.72×10^{19}	3.08×10^{9}	9.24×10^{-7}
0.001	1.72×10^{19}	1.17×10^{5}	7.70×10^{-3}
0.005	1.72×10^{19}	4.92×10^{4}	7.90×10^{-2}
0.01	1.72×10^{19}	6.69×10^{4}	1.30×10^{-1}
0.05	1.72×10^{19}	6.99×10^{3}	4.93×10^{-1}

The relationship between ECN and accuracy of BKM is shown in Table 2. From which we can see that the relation ECN $= \mathcal{O}(\varepsilon_{max}^{-1})$ still holds for problems with mixed boundary conditions. Despite of all runs in Table 2 have exactly the same condition number, we observe completely different error behaviors in cases with higher noise levels. For the noise free case, the ECN is again of the order of 10^9 even though the condition number is two order larger than that in Case 1. Once again, we see the drop in both ECN and maximum error once $\varepsilon = 0.001$ of noise is added. As the percentage of noise added to the vector b is increased, we see in Table 2 that the effective condition number decreases and maximum absolute error increases in the same order of magnitude.

4.3 Case 3: quasi-Laplace equation

If the wave number λ is sufficiently small, then the general solution for (modified) Helmholtz equations is a good approximation to that of the Laplace equation $\Delta u = 0$. In this example, the corresponding non-singular general solution (6) can also be used. In this case, analytical solution $u = 1$ is chosen. Numerical results is shown in Table 3 with different λ. We can see that the ECN is a nice indicator to the accuracy of such approximation.

4.4 Case 4: medium wave numbers

To investigate the Helmholtz problems with the medium wave numbers, consider the homogeneous Helmholtz equation on a unit square domain with analytical solution

$$u = \sin(\lambda x) + \cos(\lambda y) \tag{21}$$

Table 3: A unit square domain with only Dirichlet boundary for Case 3, number of boundary knot is 40, test boundary knot 100.

λ	Cond	ECN	ε_{max}
5.0e-8	3.31×10^{18}	8.80×10^{15}	1.78×10^{-15}
5.0e-4	5.57×10^{18}	9.56×10^{8}	2.98×10^{-7}
0.005	1.34×10^{18}	1.69×10^{7}	2.38×10^{-6}
0.05	3.54×10^{18}	1.42×10^{5}	1.70×10^{-3}

We impose Dirichlet boundary on $x = 1$ and $y = 1$ and Neumann boundary on the others. In this example, $M = 400$ test knots are randomly distributed over the region of interest. We are interested in investigating the effect of varying the number of boundary knots N.

Table 4: A unit square domain mixed boundary for case 4.

N	Cond	ECN	ε_{max}
44	1.61×10^{9}	5.92×10^{5}	8.80×10^{-3}
48	4.76×10^{11}	3.54×10^{6}	4.96×10^{-4}
52	2.00×10^{14}	2.74×10^{8}	6.43×10^{-5}
56	2.31×10^{16}	1.48×10^{9}	1.43×10^{-5}
60	4.14×10^{17}	7.39×10^{9}	2.38×10^{-7}
64	2.15×10^{17}	1.97×10^{9}	3.88×10^{-6}
68	7.77×10^{17}	4.82×10^{9}	5.19×10^{-6}

The wave number of the non-singular general solution (5) is $\lambda = 20$ for this case. The relationship between ECN of BKM and its accuracy with increasing boundary knots number is shown in Table 4. It is found that $N = 60$ boundary knots give the largest effective condition number 7.39×10^{9} corresponding with the smallest maximum error 2.38×10^{-7}. Meanwhile, $N = 60$ boundary knots can also give the largest traditional condition number 4.14×10^{17} corresponding with the same maximum error, but it is almost twice larger than the effective condition number. For boundary knot number $N > 60$, the maximum error increases as the effective condition number decreases. Thus, we may conclude that the effective condition number can be used to determine the optimal knot number with the boundary knot method to get the best numerical accuracy.

4.5 Case 5: irregular domain

As many problems are encountered on very complex physical domains in practical engineering applications, our last example considers the Helmholtz on irregular domain. (see Fig.1). Mixed boundary conditions is considered in this problem with two Neumann edges on the $x-$ and $y-$axes. Dirichlet boundary conditions are imposed on the remaining. Analytical solution is given as

$$u(x,y) = \sin(x)\cos(y). \tag{22}$$

with wave number $\lambda = \sqrt{2}$.

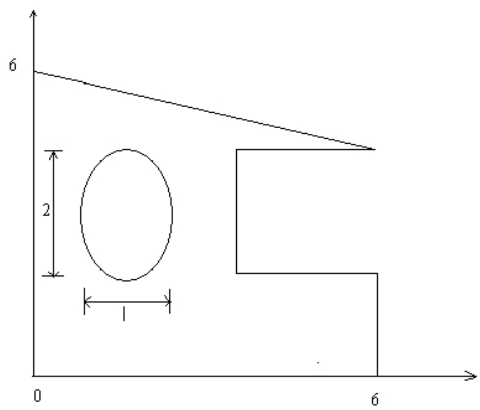

Figure 1: Configuration of 2D irregular domain for case 5.

Table 5: Fix noise level $\varepsilon = 0.00001$ with $M = 210$ test knots

N	Cond	*ECN*	ε_{max}
25	1.05×10^{12}	3.06×10^{5}	4.13×10^{-2}
33	8.51×10^{16}	9.70×10^{4}	3.37×10^{-1}
41	3.77×10^{17}	9.25×10^{4}	1.04×10^{-1}
49	5.28×10^{17}	2.04×10^{5}	1.35×10^{-2}

It is not reasonable to assume that data from real applications to be noise free. When the noise level is sufficiently small, one may solve the problem as if it is noise free. On the other hand, when the noise level is significant, some proper regularization methods should be employed. When the data is noise free, using

Table 6: Fix noise level $\varepsilon = 0.001$ with $M = 210$ test knots

N	Cond	ECN	ε_{max}
25	1.05×10^{12}	5.68×10^{3}	2.32
33	8.51×10^{16}	1.33×10^{3}	16.10
41	3.77×10^{17}	2.18×10^{3}	3.20
49	5.28×10^{17}	9.57×10^{2}	5.52

$(M,N) = (210,41)$, BKM results in a maximum accuracy of 1.42×10^{-5} with ECN 1.44×10^{9}. The author also observe that the relationship between the ECN of BKM and its accuracy is irrelevant to the numbers of boundary knots N. In Table 5 and Table 6, respectively, the maximum error and the corresponding are shown under noise levels $\varepsilon = 0.00001$ and $\varepsilon = 0.001$. Using the observations in the previous observation, one may guess that the numerical approximation will agree with the exact solution up to about one decimal place; that is good enough for many engineering problems. On the other hand, the small ECN found in Table 6 suggests that the numerical solutions are not trustworthy. In this case, one should employ regularization technique instead of applying BKM directly [Hon and Wei (2005);Wang, Chen, and Jiang (2009)].

5 Conclusions

In this study, we introduce the effective condition number to the stability analysis of the BKM. Numerical experiments strongly suggest that the effective condition number is a superior criterion over the L^2 condition number.

We also observe an underlying relationship between the effective condition number and the BKM solution accuracy. Namely, the BKM accuracy is inversely proportional to the effective condition number. More interestingly, using the effective condition number as an indicator, one can fine-tune the user-defined parameters (without the knowledge of exact solution) to ensure high accuracy from the BKM. It is revealed that when the noise level is sufficiently small, one may solve the problem as if it is noise free. On the other hand, when the noise level is significant, some proper regularization methods should be employed. All remarks above are based on numerical experiments. Theoretical study of this issue is still under way.

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