

Meshless Radial Basis Function Scheme for Problems with Boundary Singularity

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Summary

This paper introduces a meshless numerical scheme derived from radial basis functions for solving problems with boundary singularity. Since radial basis function is a continuously differentiable, positive definite and integrable function, it can easily be used to solve higher order differential equations with singularities.

Introduction to Meshless RBFs Method

The radial basis functions (RBFs) were originally devised for scattered geographical data interpolation by Hardy [1], who introduced a class of functions called multiquadric functions in the early 1970's. The basic idea of the RBFs interpolation is to approximate an unknown function, $\{f(\mathbf{x}) : \mathbf{x} \in \mathbf{R}^d\}$ by an interpolant, say $\{\hat{f}(\mathbf{x}) : \mathbf{x} \in \mathbf{R}^d\}$ at a set of N distinct data points $X = \{\mathbf{x}_j : j = 1, 2, \dots, N\}$. Let $\Phi : \mathbf{R}_+ \rightarrow \mathbf{R}$ be a set of positive definite basis functions defined by $\Phi = \phi(\|\mathbf{x} - \mathbf{x}_j\|)$ on a fixed space \mathbf{R}^d . Here $\phi(\|\mathbf{x} - \mathbf{x}_j\|)$ is referred to a typical type of RBFs solely dependent on the Euclidean distance between \mathbf{x} and a fixed point $\mathbf{x}_j \in \mathbf{R}^d$.

The general form of RBFs interpolant to a function $f(\mathbf{x})$ can be expressed in the form of a finite series

$$\hat{f}(\mathbf{x}) = \sum_{j=1}^N \alpha_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{k=1}^L b_k p_k(\mathbf{x}) \quad \mathbf{x} \in \mathbf{R}^d, \quad 0 < L \ll N, \quad (1)$$

where the term $\{p_k(\mathbf{x}) | k = 1, 2, \dots, L\}$ is a basis of polynomial and α_j 's and b_k 's are the unknown coefficients. The approximation function in (1) has a unique solution if the system satisfies the conditions $\hat{f}(\mathbf{x}_i) = f(\mathbf{x}_i)$ and the constraints $\sum_{j=1}^N \alpha_j p_k(\mathbf{x}_j) = 0$, for $i = 1, 2, \dots, N$, $k = 1, 2, \dots, L$, for $L \ll N$. This yields a system of linear equations, which can be expressed in matrix form $[\mathbf{M}_\phi] \vec{\alpha} = \vec{\mathbf{Y}}$, where $[\mathbf{M}_\phi]$ is a square matrix, $\vec{\alpha}$ and $\vec{\mathbf{Y}}$ are column matrices. Since each RBF, $\phi \in \mathbf{R}^d$ is positive definite, the matrix $[\mathbf{M}_\phi]$ is non-singular so the linear system has a unique solution. The unknown coefficients α_j 's and b_k 's can also be obtained uniquely by solving the linear system. In other words, the non-singularity of the interpolation matrix $[\mathbf{M}_\phi]$ can be guaranteed, provided the matrix $[\mathbf{M}_\phi]$ is positive definite for all sets of distinct centers $X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\} \in \mathbf{R}^d$.

A general theory on the existence, uniqueness and convergence of the RBFs interpolation was proven by Micchelli [2] in 1986. Micchelli's result was extended by Powell [3],

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and Wu *et al* [4] to deduce some important non-singularity properties of the RBFs interpolation. There are many possible radial basis functions. The most commonly used has been the multiquadric function, reciprocal multiquadric, thin plate splines and Gaussian.

Application to Boundary Value Problems with Singularities

The present paper illustrates a class of meshless RBFs method, which possesses a simple mathematical formulation and high order of convergence, to solve problems with singularity. Motz's problem is used as a reference test to illustrate the numerical performance. This problem was first study by Motz [5] in 1947 using the finite difference scheme together with the relaxation method. Whiteman [6] *et al* in 1972 extended the study using the conformal transformation method. Thatcher [7] in 1976 made use of infinite grid refinement to deal with singularities. Most recently, Li [8] in 1998 studied the problem extensively with conformal mappings and some combined methods.

The problem deal with the Laplace equation $\nabla^2 u = 0$, over a square region satisfying the mixed Neumann and Dirichlet boundary conditions as indicated in Figure 1(a). The singular point occurred at the crack tip produces discontinuity of the solution at the origin.

The solution of Motz's problem has been found to be anti-symmetric over a unit square. This leads to have the transformation $v = (u - 500)$, which only requires to solve the upper-half of the square plate Ω_u . The transformed problem is defined on $\Omega_v = \{(x, y), -\frac{L}{2} \leq x \leq \frac{L}{2}, 0 \leq y \leq \frac{L}{2}\}$ as depicted in Figure 1(b). Thus, the transformed Motz's problem and its boundary conditions can be re-written as

$$\nabla^2 v = 0, \text{ in } \Omega_v \setminus \partial\Omega_v \subset \mathbf{R}^2 \quad (2)$$

subject to the following boundary conditions

$$\begin{aligned} \Gamma_1 : \frac{\partial v}{\partial x} &= 0 \text{ for } x = -\frac{L}{2}, 0 \leq y \leq \frac{L}{2}; & \Gamma_2 : \frac{\partial v}{\partial y} &= 0 \text{ for } -\frac{L}{2} \leq x \leq \frac{L}{2}, y = \frac{L}{2}; \\ \Gamma_3 : \frac{\partial v}{\partial y} &= 0 \text{ for } y = 0, 0 \leq x \leq \frac{L}{2}; & \Gamma_4 : v &= 0 \text{ for } -\frac{L}{2} \leq x \leq 0, y = 0; \\ \Gamma_5 : v &= 500 \text{ for } x = \frac{L}{2}, 0 \leq y \leq \frac{L}{2}. \end{aligned}$$

According to the analysis of singularity from Motz [5] the local analytic solution $v_h(x)$ in the vicinity of the singular point can be modelled by the following series expansion

$$(r, \theta) : v_h(r, \theta) = \sum_{i=1}^{\infty} A_i r^{i-\frac{1}{2}} \cos[(i-1/2)\theta], \quad (3)$$

where A_i are the expansion coefficients, and (r, θ) is the polar coordinates of the neighbouring point about the origin. The next section describes the application of the computational procedures.

Computational Procedure and Numerical Results

To handle the boundary singularity in the neighbourhood of the singular point, the

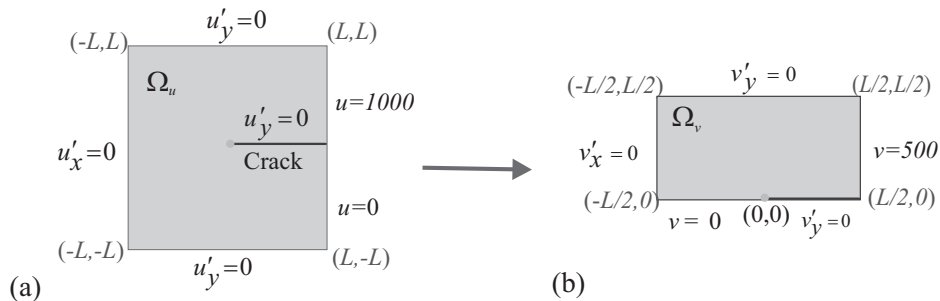


Figure 1: (a) The original Motz's problem, (b) Transformed problem and its boundary conditions

involved domain $\Omega_v \subset \mathbf{R}^2$ is divided into two non-overlapping subdomains Ω_{v_1} and Ω_{v_2} such that $\Omega_v = \Omega_{v_1} \cup \Omega_{v_2}$. The subdomain Ω_{v_2} as shown in Figure 2(b) is the open upper-half disk with radius r_s , which covers the origin that forms the boundary singularity.

Let $X_1 = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{N_{int}}\} \subset \mathbf{R}^2$ in $\Omega_{v_1} \setminus \partial\Omega_v$ and $X_2 = \{\mathbf{x}_{N_{int}+1}, \dots, \mathbf{x}_N\} \in \mathbf{R}^2$ in $\partial\Omega_v$ be a set of distinct interior and boundary nodal points respectively, where N is the total number of collocation points over the subdomain Ω_{v_1} such that $N = (N_{int} + \sum_{i=1}^5 N_{\Gamma_i})$, N_{int} stands for the number of interior nodal points and N_{Γ_i} stands for the number of nodal points on boundary Γ_i , for $i = 1, 2, 3, 4, 5$. These points are selected to coincide with the collocation points over the subdomain Ω_{v_1} . By collocating at the same set of nodal points $(x_i, y_i)_{i=1}^N$ from X_1 and X_2 , the RBFs interpolant for the solution to equation (2) is given by

$$v_h(x, y) = \sum_{j=1}^N \alpha_j \phi(r_j) + \beta_1 x + \beta_2 y + \beta_3, \text{ in } \Omega_v \quad (4)$$

subject to the following three linear conditions

$$\sum_{i=1}^N \alpha_i x_i = \sum_{i=1}^N \alpha_i y_i = \sum_{i=1}^N \alpha_i = 0, \quad (5)$$

such that the coefficients of β_1 , β_2 and β_3 of equation (4) can be determined uniquely. The unknown coefficients α_j 's and β_1 , β_2 , β_3 are to be determined by collocating N distinct scattered points $\{(x_j, y_j)\}_{j=1}^N$. In this example, the basis function $\phi(r_j)$ is taken to be the classical multiquadric radial basis function (MQ-RBFs), which is defined by $\phi(r_j) = \sqrt{(x-x_j)^2 + (y-y_j)^2 + \delta_j^2}$, for $j = 1, 2, \dots, N$, where δ_j^2 is the shape parameter. The magnitude of the shape parameters δ_j is a key factor for obtaining accurate solution. The effect of the shape parameter has been reported in several references, such as in [9]. This study observed that the optimal solutions can be achieved by setting $\delta_j = C$ as a constant between $0.65 \leq C \leq 0.9$.

Differentiating equation (4) with respect to x and y yields the required partial derivatives $\frac{\partial^2 v_h}{\partial x^2}$ and $\frac{\partial^2 v_h}{\partial y^2}$. The unknown coefficients α'_j 's and $\beta_1, \beta_2, \beta_3$ can be determined by substituting these partial derivatives into the equation (2), which yields the following system

$$\sum_{j=1}^N \alpha_j \left[\frac{[1 - M_x^2]}{\phi(r_{i,j})} + \frac{[1 - M_y^2]}{\phi(r_{i,j})} \right] = 0, \quad \text{in } \Omega_{v_1} \setminus \partial\Omega_v \quad (6)$$

for the interior points $i = 1, \dots, N_{int}$, where $M_x = (x_i - x_j) / \phi(r_{i,j})$, $M_y = (y_i - y_j) / \phi(r_{i,j})$ and $\phi(r_{i,j})$ is the chosen radial basis function. The specific boundary conditions in Γ'_i 's are approximated by

$$\left. \begin{aligned} \sum_{j=1}^N \alpha_j M_x + \beta_1 &= 0; (x_i, y_i) \in \Gamma_1, \\ \sum_{j=1}^N \alpha_j M_y + \beta_2 &= 0; (x_i, y_i) \in \Gamma_2 \cup \Gamma_3; \\ \sum_{j=1}^N \alpha_j \phi(r_{i,j}) + (\beta_1 x_i + \beta_2 y_i + \beta_3) &= 0; (x_i, y_i) \in \Gamma_4; \\ \sum_{j=1}^N \alpha_j \phi(r_{i,j}) + (\beta_1 x_i + \beta_2 y_i + \beta_3) &= 500; (x_i, y_i) \in \Gamma_5. \end{aligned} \right\} \quad (7)$$

Once the coefficients are determined, the approximate solutions $v_h(x_i, y_i)$ in Ω_1 can be calculated. We now turn to consider the treatment of the singularity at the origin. Let N_d be the number of distinct nodal points inside Ω_{v_2} , which are close to the singular point. The solutions v_h in Ω_{v_2} are calculated by using the series expansion in equation (3) which yields the expression

$$v_h(r, \theta) = \sum_{m=1}^{N_d} A_m r^{m-\frac{1}{2}} \cos(m-1/2)\theta, \quad \text{in } \Omega_{v_2}. \quad (8)$$

This paper incorporates with the least square approximation method to calculate the best fit for coefficients $\{A_j : j = 1, 2, \dots, N_d\}$ of the series expansion. To do this, we choose $(N_d + l)$ nodal points inside the subdomain Ω_{v_2} , where $l \geq 3$. These nodal points have a one-one correspondence between their polar coordinates and their Cartesian coordinates: $(r_k, \theta_k) \Leftrightarrow (x_k, y_k)$, where $x_k = r_k \cos \theta_k$ and $y_k = r_k \sin \theta_k$, for $k = 1, \dots, (N_d + l)$. We take $l = 3$ in this study. The sum of squares of the error between $v_h(x_k, y_k)$ and $v_h(r_k, \theta_k)$ are given by

$$S = \sum_{(x_k, y_k)} \left[v_h(x_k, y_k) - \left(\sum_{m=1}^{N_d} A_m r_k^{m-\frac{1}{2}} \cos(m-1/2)\theta_k \right) \right]^2. \quad (9)$$

The best fitted coefficients A'_m 's can be determined by minimizing S , the sum of the squares of the error, hence

$$\frac{\partial S}{\partial A_m} = 0, \quad \text{for } m = 1, 2, \dots, N_d. \quad (10)$$

In the computation, we organized equations (5), (6), (7) and (10) into a matrix form, $[M][\vec{a}] = [\vec{p}]$, where $[M]$ has order $(N + 3 + N_d) \times (N + 3 + N_d)$, $[\vec{a}]$ and $[\vec{p}]$ are $(N + 3 + N_d)$ column vectors. As mention previously, MQ-RBFs is positive definite and continuously differentiable, the resulting matrix $[M]$ is conditionally positive definite and hence invertible. Once the unknown coefficients are determined, we can proceed to calculate the approximation solution $v_h(x_i, y_i)$ accordingly by using equation (4) and (8).

The numerical results are compared with those from the reference book presented by Li [8], where the author used boundary approximation method to evaluate the values with double precision. In the present numerical experiment, the numerical results are generated in double precision and the numerical accuracy is found to be seriously affected by the large condition number of the full coefficient matrix $[M]$. The maximum relative errors of the approximate solutions is about 5.30E-02 when 261 collocation points are selected. Figure3(a) depicted the approximate solution v'_h 's over the entire domain and Figure 3(b) illustrates the approximate solution v'_h 's at three specific nodal points at $y = 0.3, 0.5$ and 0.8 . It can be observed from these figures that the proposed method produce a reasonable degree of accuracy, which indicates a good performance of using the MQ-RBFs method in the given model.

In summary, the important shortcoming of the global MQ-RBFs method is the poor condition number, which has seriously hindered its ability from solving the system with a large number of nodal points. This property makes the model to produces a rather weak approximation in the region with Neumann boundary condition. However, this shortcoming can be handled by using domain decomposition scheme when solving problems with a large system of equations. The authors of this paper is currently investigating the numerical performance of domain decomposition with RBFs method. The preliminary results have been shown to be very effective to overcome the shortcoming of RBFs method problem.

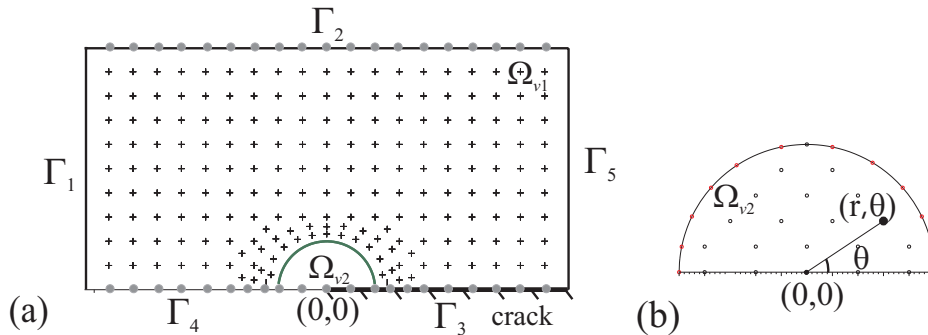


Figure 2: (a) Collocation points on subdomain Ω_{v1} , (b) Collocation points inside the upper half disk Ω_{v2} with $0 < \theta < \pi, 0 < r < r_s$

Acknowledgment This research is supported by the Research and Development Fund of the Open University of Hong Kong, No. 03/1.2 and Research Grants Council of the Hong Kong Special Administrative Region, China (Project No. CityU 1178/02P).

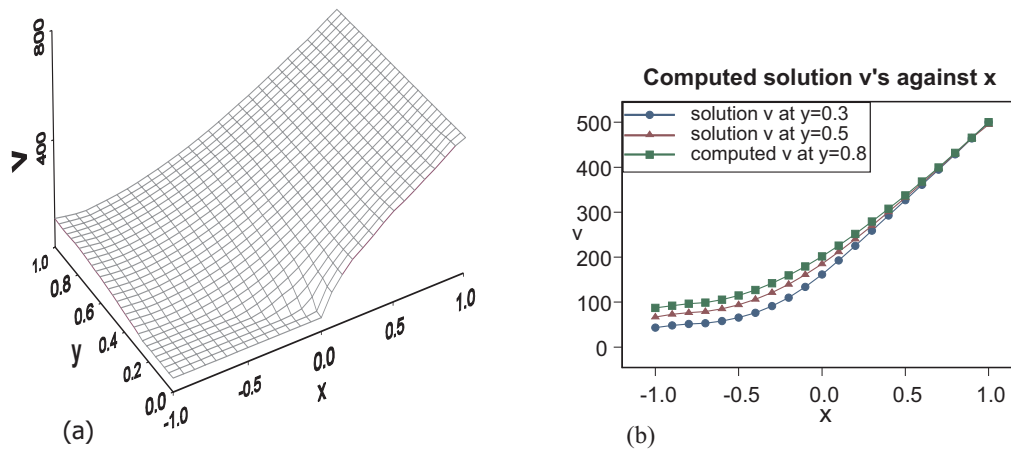


Figure 3: (a) The solution of $v_h(x, y)$ over entire domain Ω_v , (b) The solution $v_h(x, y)$ at three nodal points $y = 0.3, 0.5$ and 0.8 .

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