

Solving the singular Motz problem using Radial Basis functions

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Abstract

Mathematical model has been used extensively in solving engineering problems with singularity. This paper introduces a mesh-free numerical scheme for solving problems with boundary singularity. The solution of the governing equation is approximated by a class of mesh-free radial basis functions. The proposed radial basis function is a continuously differentiable, positive definite and integrable function, it can easily be used to solve higher order of differential equations. In the vicinity of the singular point, we use a series to approximate the solution. Then domain decomposition is used to blend the two solutions together.

Keywords: Radial basis functions, singular problem, domain decomposition.

Introduction

The behaviour of many fatigue and fracture mechanics can be modelled as problems with boundary singularity. Studies of boundary singularity problems can be traced back to Motz [1] in 1946. The author adopted the classical finite difference scheme together with the relaxation method to overcome the discontinuity occurring from the crack tip over the boundary interface. The solution to the Motz's problem is singular at the origin and is often used by many researchers as reference example for testing numerical methods. The Motz's problem has the form $\nabla^2 u = -f$, where f is a specific function. In the vicinity of the singular point, the singular solutions u can be written as $u = \hat{u}_h + u_p$, where \hat{u}_h is the homogeneous solution and u_p is the particular solution. For the two-dimensional Laplace equations, the homogeneous solution \hat{u}_h in the vicinity of the singular points can be found in [2] and is given by the asymptotic series of the form

$$u_h = \sum_{i=1}^{\infty} A_i r^{\alpha_i} f_i(\theta), \quad r, \theta \in \Omega$$

over a connected region Ω , where A_i are the unknown expansion coefficients to be determined. These coefficients are termed as generalized flux intensity factors (GFIFs). The polar coordinates (r, θ) centred at the singular point and (α_i, f_i) associated with eigen-pairs, where α_i is the power arranged in ascending order as defined by $\alpha_i \leq \alpha_{i+1}$.

Yosibash *et al* [3, 4] in 1997 developed a mesh-dependent method derived from the least-square finite difference scheme for approximating solutions in the vicinity of the singular point and a conventional finite difference scheme was then applied to the remaining part of the given problem. Another comprehensive study on crack tip analysis of singularity problems was carried out by Li [5] using conformal mappings and several types of combined methods.

Recently Rao *et al* [6] developed an element-free Galerkin method (EFGM) for fracture analysis of cracks. However, the mathematical formulation is rather complicated and consists of three components: (i) moving least-squares approximation; (ii) choosing the weight functions and (iii) variational formulation and discretization. This paper introduces an efficient mesh-free numerical scheme which is derived from a class of radial basis functions (RBF). The RBF method possess a simple mathematical formulation and a truly mesh free property, which does

not require a global mesh for supporting computations. In addition, RBF are continuously differentiable and integrable, and is insensitive to dimension d . These features make it suitable for solving problems in higher dimensions with unsmooth boundary conditions.

Meshless Radial Basis Function Method for Solving PDEs

This paper discusses a mesh free approximation scheme based on the radial basis function for solving the problems with complex boundary conditions and singularities. The RBF methods have been found to have major advantages over the classical finite element or finite difference methods. One of these advantages is that it does not require the construction of an underlying mesh. This allows it to handle complicated boundaries with concave surface more efficiently. The basic concept of the RBF method is described below.

The RBFs were originally devised for scattered geographical data interpolation by Hardy [7], who introduced a class of functions called multiquadric functions in the early 1970's. The basic idea of the RBF interpolation is to approximate an unknown function, $\{f(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^d\}$ by an interpolant, say $\{\hat{f}(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^d\}$ at a set of N distinct data points $X = \{\mathbf{x}_j : j = 1, 2, \dots, N\}$. Let $\Phi : \mathbb{R}_+ \rightarrow \mathbb{R}$ be a set of positive definite basis functions defined by

$$\Phi = \{\phi(\|\mathbf{x} - \mathbf{x}_j\|)\}, \quad \mathbf{x}, \mathbf{x}_j \in \mathbb{R}^d$$

on a fixed space \mathbb{R}^d . Here $\phi(\|\mathbf{x} - \mathbf{x}_j\|)$ refers to a typical type of RBFs that is solely dependent on the Euclidean distance between \mathbf{x} and a fixed point $\mathbf{x}_j \in \mathbb{R}^d$. The RBF interpolant to the approximated solution of $f(\mathbf{x})$ can be expressed as a finite linear combination of $\phi(\|\mathbf{x} - \mathbf{x}_j\|)$:

$$\hat{f}(\mathbf{x}) = \sum_{j=1}^N \alpha_j \phi(\|\mathbf{x} - \mathbf{x}_j\|), \quad \mathbf{x}, \mathbf{x}_j \in \mathbb{R}^d, \quad (1)$$

where $\{\alpha_j : j = 1, 2, \dots, N\}$ are the unknown coefficients, which can be determined by setting the following condition:

$$\hat{f}(\mathbf{x}_i) = f(\mathbf{x}_i), \quad i = 1, 2, \dots, N. \quad (2)$$

This yields a system of linear equations, which can be expressed in the following matrix form

$$[\mathbf{A}_\phi] \vec{\alpha} = \vec{\mathbf{F}}, \quad (3)$$

where $[\mathbf{A}_\phi] = [\phi(\mathbf{x}_i - \mathbf{x}_j)]_{1 \leq i, j \leq N}$ is an $N \times N$ matrix, $\vec{\alpha} = [\alpha_1, \alpha_2, \dots, \alpha_N]^T$ and $\vec{\mathbf{F}} = [f(\mathbf{x}_1), f(\mathbf{x}_2), \dots, f(\mathbf{x}_N)]^T$ are $N \times 1$ column matrices. Provided that the chosen radial basis function $\phi \in \mathbb{R}^d$ is positive definite, the matrix $[\mathbf{A}_\phi]$ is non-singular so the linear system (3) has a unique solution. The unknown coefficients $\{\alpha_j\}$ can be obtained uniquely by solving the linear system (3).

Although the above-mentioned condition guarantees the uniqueness of some particular RBF interpolants, not all RBFs can satisfy the conditions of positive definiteness. A general theory on the existence, uniqueness and convergence of the RBFs interpolation was proven by Micchelli [8] in 1986. In accordance with the Micchelli's result, Powell [9], Madych *et al* [10] and Wu *et al* [11] extended the study and deduced some important non-singularity properties of the RBF interpolation. Their analysis concluded that the RBF interpolation method possess a super-convergent property and truly mesh-free algorithm. The RBF method has been demonstrated to be highly flexible for the approximation of high spatial dimensional problems. The accuracy of the RBF interpolant has an order of convergence $\mathcal{O}(h^{d+1})$, where h is the density of the

collocation points and d is the spatial dimension.

Many of RBF ideas can be easily generalized to the case where the basis function ϕ is only conditionally positive definite [12] in which one needs to add a finite number of polynomial of suitable degree to the interpolant $\hat{f}(\mathbf{x})$ in equation (1) and impose additional conditions to accomplish its uniqueness. Let $Q_m^d(\mathbf{x}) \in \Pi_m$ where Π_m is a set of d -variate polynomials of degree less than m . The RBF interpolant $\hat{y}(\mathbf{x})$ is now written as

$$\hat{f}(\mathbf{x}) = \sum_{j=1}^N \alpha_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + Q_m^d(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad 0 < m < N, \quad (4)$$

where

$$Q_m^d(\mathbf{x}) = \sum_{k=1}^L b_k p_k(\mathbf{x}), \quad L = \frac{(m+d-1)!}{(m-1)!d!}.$$

The terms $\{p_k(\mathbf{x}) \mid k = 1, 2, \dots, L\}$ are the basis of $Q_m^d(\mathbf{x})$. The approximation function of (4) has a unique solution if the system satisfies the conditions (2) and the following constraints

$$\sum_{j=1}^N \alpha_j p_k(\mathbf{x}_j) = 0, \quad k = 1, 2, \dots, L. \quad (5)$$

Note that, in this case, the matrix $[\mathbf{A}_\phi]$ is enlarged to order $(N+L) \times (N+L)$, and $\vec{\alpha}$ and $\vec{\mathbf{Y}}$ are $(N+L) \times 1$ column matrices. Although there are many possible radial basis functions, the followings are the most popular choices:

$$\phi(r_j) = \begin{cases} r_j^3, & \text{Cubic} & (a) \\ (r_j^2) \log r_j, & \text{Thin plate splines in } R^2 & (b) \\ e^{-\sigma r_j^2}, & \text{Gaussian, } \sigma > 0 & (c) \\ (r_j^2 + \delta^2)^{\frac{1}{2}}, & \text{Multiquadric, } \delta \in R & (d) \\ (r_j^2 + \delta^2)^{-\frac{1}{2}}, & \text{Reciprocal multiquadric, } \delta \in R & (e) \end{cases} \quad (6)$$

where $\{r_j = \|\mathbf{x} - \mathbf{x}_j\| \mid j = 1, 2, \dots, N\}$ is the Euclidean distance between \mathbf{x} and $\mathbf{x}_j \in \mathbb{R}^d$ and $\delta^2 \in \mathbb{R}$ is the shape parameter of the multiquadric functions in (d) & (e), which is used to control the fitting of a smooth surface to the data. These functions are globally supported and will generate a system of equations with a full matrix. However, as shown by Madych and Nelson [13], the multiquadric function (MQ-RBF) can be exponentially convergent so we can often use a relatively small number of basis elements to achieve a computational efficiency. As a consequence, the MQ-RBF method has been the most commonly used has been radial basis function and progressively refined recently by Kansa [14] and widely used by Hon *et al* [15] and Wong *et al* [16] to solve scientific and engineering problems. Their results from solving elliptic, parabolic and hyperbolic problems were shown to be better than other well established approximation methods.

The Algorithm

To study the performance of the proposed method, we apply it to solve a classical re-entrant corner problem. Re-entrant corner problem possesses a typical nature of singularity of solution, the singular point occurs at the origin forming an angle of $\gamma\pi$ which would result discontinuity. The model involves the Laplace equation satisfying some mixed Neumann and Dirichlet

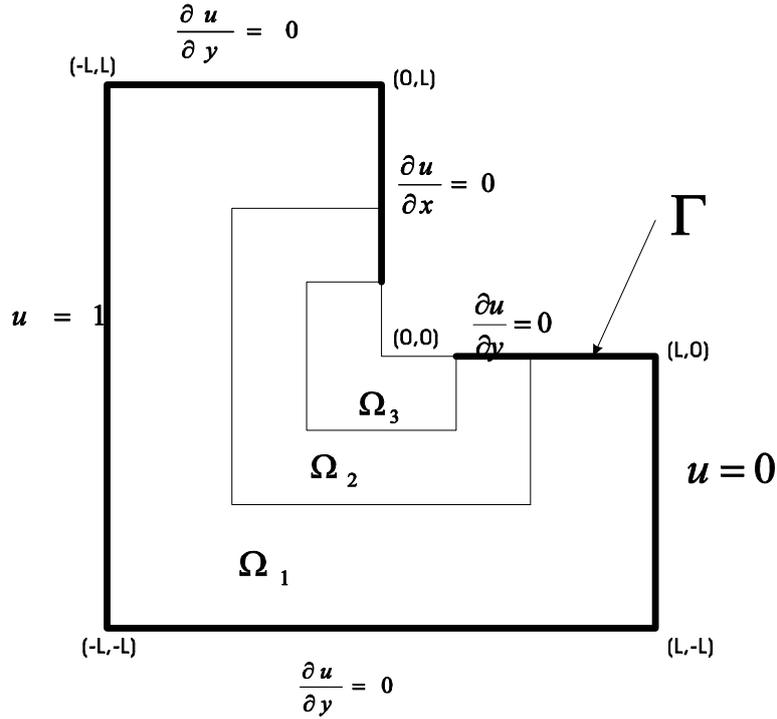


Figure 1: A region with an re-entrance angle.

boundary conditions. The re-entrant corner with the L-shaped domain as depicted in Figure (1), is a special case in which, $\gamma = \frac{3}{2}\pi$ at the origin.

The governing equation is:

$$\nabla^2 f = 0 \quad (7)$$

and the boundary conditions are depicted in the figure. We then divide the region into three as shown in the figure. Ω_1 is the region that is far away from the corner and Ω_3 is the region close to the the corner. Ω_2 is the region between Ω_1 and Ω_3 . We are going to use a radial basis function to approximate the solution in Ω_1 and Ω_2 and the series solution to approximate the solution in Ω_2 and Ω_3 .

Let $X_1 = \{\mathbf{x}_i | i = 1, \dots, N_1\}$ be nodes in Ω_1 , $X_2 = \{\mathbf{x}_i | i = N_1 + 1, \dots, N_1 + N_2\}$ be nodes on the boundary Γ in the figure, $X_3 = \{\mathbf{x}_i | i = N_1 + N_2 + 1, \dots, N_1 + N_2 + N_3\}$ be nodes in Ω_2 . We now use these $N (= N_1 + N_2 + N_3)$ nodes in forming the approximation of the solution:

$$f_{rbf}(\mathbf{x}) = \sum_{j=1}^N a_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{j=1}^M b_j p_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad 0 < M < N.$$

For solution close to the re-entrance corner, we would approximate the solution using the series solution:

$$f_{series}(r, \theta) = \sum_{i=1}^P c_i r^{\frac{2}{3}(i-1)} \cos \left[\frac{2}{3}(i-1)\theta \right], \quad -3\pi/2 \leq \theta \leq 0. \quad (8)$$

For each of the node in X_1 , we would set up an equation according to (7), so we have N_1 equations for them:

$$[\mathbf{A} \quad \mathbf{B}] \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = [\mathbf{0}], \quad (9)$$

where \mathbf{A} is an $N_1 \times N$ matrix, \mathbf{B} is an $N_1 \times M$ matrix, \mathbf{a} is an $N \times 1$ matrix, \mathbf{b} is an $M \times 1$ matrix, and

$$\begin{aligned} \{\mathbf{A}\}_{ij} &= \nabla^2 \phi(\|\mathbf{x} - \mathbf{x}_j\|) \Big|_{\mathbf{x}=\mathbf{x}_i}, \\ \{\mathbf{B}\}_{ij} &= \nabla^2 p_j(\mathbf{x}) \Big|_{\mathbf{x}=\mathbf{x}_i}, \\ [\mathbf{a}] &= \{a_1, \dots, a_N\}^T, \\ [\mathbf{b}] &= \{b_1, \dots, b_M\}^T. \end{aligned}$$

Let the boundary condition be specified as:

$$B_{ou}(f) = v(\mathbf{x}), \text{ for } \mathbf{x} \in \Gamma, \quad (10)$$

where B_{ou} is the boundary condition operator and $v(\mathbf{x})$ is the prescribed boundary condition. So for each node in X_2 , we would set up an equation according to (10):

$$[\mathbf{C} \quad \mathbf{D}] \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = [\mathbf{d}], \quad (11)$$

where \mathbf{C} is an $N_2 \times N$ matrix, \mathbf{D} is an $N_2 \times M$ matrix, and

$$\begin{aligned} \{\mathbf{C}\}_{ij} &= bou(\phi(\|\mathbf{x} - \mathbf{x}_j\|)) \Big|_{\mathbf{x}=\mathbf{x}_{i+N_1}}, \\ \{\mathbf{D}\}_{ij} &= bou(p_j(\mathbf{x})) \Big|_{\mathbf{x}=\mathbf{x}_{i+N_1}}, \\ [\mathbf{d}] &= \{v(\mathbf{x}_{1+N_1}), \dots, v(\mathbf{x}_{N_2+N_1})\}^T. \end{aligned}$$

For nodes in X_3 we would we would set up an equation so that the radial basis solution equals to that of the series solution:

$$[\mathbf{E} \quad \mathbf{F} \quad \mathbf{G}] \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{bmatrix} = [\mathbf{0}], \quad (12)$$

where \mathbf{E} is an $N_3 \times N$ matrix, \mathbf{F} is an $N_3 \times M$ matrix, \mathbf{E} is an $N_3 \times P$ matrix, and

$$\begin{aligned} \{\mathbf{E}\}_{ij} &= \nabla^2 \phi(\|\mathbf{x} - \mathbf{x}_j\|) \Big|_{\mathbf{x}=\mathbf{x}_{i+N_1+N_2}}, \\ \{\mathbf{F}\}_{ij} &= \nabla^2 p_j(\mathbf{x}) \Big|_{\mathbf{x}=\mathbf{x}_{i+N_1+N_2}}, \\ \{\mathbf{G}\}_{ij} &= -r^{\frac{2}{3}(j-1)} \cos \left[\frac{2}{3}(j-1)\theta \right] \Big|_{r=r_{i+N_1+N_2}, \theta=\theta_{i+N_1+N_2}}, \\ [\mathbf{c}] &= \{c_1, \dots, c_P\}. \end{aligned}$$

Then, we select additional nodes $X_4 = \{x_{N_1+N_2+N_3+1}, \dots, x_{N_1+N_2+N_3+N_4}\}$ in Ω_2 so that $N_4 >$

P , we would then use the least square method to set up the last P equations. First we find the sum of square of differences between the radial basis function and the series solution at nodes in X_4 :

$$S = \sum_{j=1}^{N_4} (f_{rbf}(\mathbf{x}) - f_{series}(r, \theta))^2.$$

Then, we would set up one equation for each of

$$\frac{\partial S}{\partial c_i} = 0, \text{ for } i = 1, \dots, P. \quad (13)$$

In matrix form, (13) is:

$$\begin{bmatrix} \mathbf{K}^T \mathbf{H} & \mathbf{K}^T \mathbf{J} & \mathbf{K}^T \mathbf{K} \end{bmatrix} \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{bmatrix} = [\mathbf{0}], \quad (14)$$

where \mathbf{H} is an $N_4 \times N$ matrix, \mathbf{J} is an $N_4 \times N$ matrix, \mathbf{K} is an $N_4 \times P$ matrix, and

$$\begin{aligned} \{\mathbf{H}\}_{ij} &= \nabla^2 \phi(\|\mathbf{x} - \mathbf{x}_j\|) \Big|_{\mathbf{x}=\mathbf{x}_{i+N_1+N_2+N_3}}, \\ \{\mathbf{J}\}_{ij} &= \nabla^2 p_j(\mathbf{x}) \Big|_{\mathbf{x}=\mathbf{x}_{i+N_1+N_2+N_3}}, \\ \{\mathbf{K}\}_{ij} &= -r^{\frac{2}{3}(j-1)} \cos \left[\frac{2}{3}(j-1)\theta \right] \Big|_{r=r_{i+N_1+N_2+N_3}, \theta=\theta_{i+N_1+N_2+N_3}}. \end{aligned}$$

We can then combine all the equations (9), (11), (12) and (14), we have the following system

$$\mathbf{LP} = \mathbf{Q}, \quad (15)$$

where

$$\mathbf{L} = \begin{bmatrix} \mathbf{A} & \mathbf{B} & \mathbf{0} \\ \mathbf{C} & \mathbf{D} & \mathbf{0} \\ \mathbf{E} & \mathbf{F} & \mathbf{G} \\ \mathbf{K}^T \mathbf{H} & \mathbf{K}^T \mathbf{J} & \mathbf{K}^T \mathbf{K} \end{bmatrix}, \mathbf{P} = \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \\ \mathbf{c} \end{bmatrix}, \text{ and } \mathbf{Q} = \begin{bmatrix} \mathbf{0} \\ \mathbf{d} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}.$$

The solution of \mathbf{P} from (15) can be obtained by

$$\mathbf{P} = \mathbf{L}^{-1} \mathbf{Q}.$$

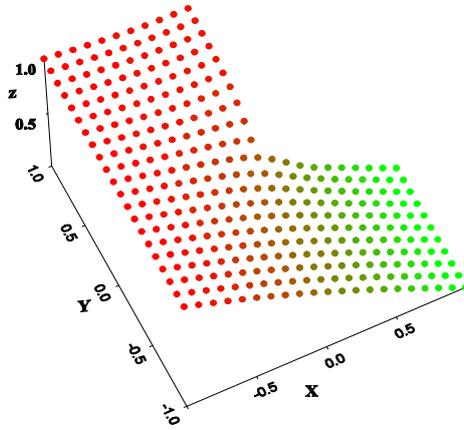
Numerical Results

The numerical results from the proposed scheme are compared with that obtained by Yosibash [3], who produced the value of A_i by using finite element method. The computational results for u 's were generated 342 collocation points over the domain Ω_u . Table 1 analyses the first four intensity factors c_1, c_2, c_3 and c_4 of the series expression (8).

Table 1

Intensity factors	Results from Yosibash [3]	Results from MQ-RBF Method
c_1	0.6667	0.6676
c_2	-0.4520	-0.4514
c_3	-0.2149	-0.2139
c_4	0.0000	4.1516×10^{-5}

The maximum relative errors of the approximate results is $5.30\text{E-}02$ when comparing to the global solution obtained from series expansion. The small magnitude of relative errors reflects the proposed radial basis function method to produce a reasonable degree of accuracy. Figure 2 shows the predicted results over Ω_u of the underlying problem. The smooth distribution indicates a good performance of using the RBF method in the given model.

Figure 2: Predicted result of $u(x, y)$ over the L-sharp region.

From the numerical experience, we observed that the results of MQ-RBF method appear to have a same order of magnitude as those results achieved by Yosibash [3], where the authors reported that their first four coefficients are accurate up to the shown 4 decimal places. Our results indicates that the RBF method combined with overlapping domain decomposition is not only an efficiency scheme, it also produced a high level of accurate approximation. The present scheme has been shown to be very effective to overcome the shortcoming of RBF method as mentioned above.

Conclusions

In summary, the MQ-RBF method used in this paper is type of globally supported functions. The disadvantage of such global RBF is that the result in a full matrix which is computationally expensive and may cause instability if the matrix is ill-conditioned, which has seriously hindered its ability from solving large scale problem with a large number of nodal points. This shortcoming leads to the studies of domain decomposition scheme. The combination of RBF scheme and domain decomposition has been verified to be a very effective technique to overcome this shortcoming of RBF method. The overlapping domain decomposition scheme used in this paper is specially designed to overcome the discontinuity of the solution near the singular point. The special region which covers the singular point, is small and Ω_{12} is common region to both Ω_1 and Ω_2 .

On the other hand, the RBF method possesses a number of attractive properties. The greatest attractive properties are the mesh free configuration and the simple mathematical formulation, these properties make the RBF method more flexible in coupling with other remedial numerical schemes. In this paper, we would easily incorporate the domain decomposition and least square approximation scheme with RBF. We showed that the least square approximation with MQ-RBF lead to a small numerical discrepancy in the numerical experiments.

We have illustrated the efficiency of the proposed scheme. However, the scheme can be applied to any elliptic problems with boundary singularity, provided that the solution in the vicinity of the singular point in the form of asymptotic series expansion has been known explicitly. In addition, since the RBF method is insensitive to the dimension of the problem, the scheme can be used to solve higher dimensional problems.

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