Localized Meshfree Methods for Solving 3D-Helmholtz Equation

Reza Mollapourasl, Majid Haghi

Abstract—In this study, we develop local meshfree methods known as radial basis function-generated finite difference (RBF-FD) method and Hermite finite difference (RBF-HFD) method to design stencil weights and spatial discretization for Helmholtz equation. The convergence and stability of schemes are investigated numerically in three dimensions with irregular shaped domain. These localized meshless methods incorporate the advantages of the RBF method, finite difference and Hermite finite difference methods to handle the ill-conditioning issue that often destroys the convergence rate of global RBF methods. Moreover, numerical illustrations show that the proposed localized RBF type methods are efficient and applicable for problems with complex geometries. The convergence and accuracy of both schemes are compared by solving a test problem.

Keywords—Radial basis functions, Hermite finite difference, Helmholtz equation, stability.

I. INTRODUCTION

THE 3-D Helmholtz equation considered in this work is expressed as

$$\nabla^2 u(\mathbf{x}) + k^2 u(\mathbf{x}) = f(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \tag{1}$$

$$u(\mathbf{x}) = \bar{u}(\mathbf{x}), \qquad \mathbf{x} \in \Gamma \tag{2}$$

where ∇^2 is the Laplacian operator, k is the wave number, unknown u usually represents a pressure field in the frequency domain, f denotes the source function and $\bar{u}$ is a known function on $\Gamma = \partial\Omega$.

All acoustic radiation problems can be modeled as the wave equation subject to certain initial and boundary conditions. For a constant frequency case, the problem reduces to solving the Helmholtz equation (1), subject to certain boundary conditions. The Helmholtz equation sounds simple but in reality the analytic solution to the Helmholtz equation exists only for certain types of source geometry that the Helmholtz equation is separable. In most engineering applications the source geometry is arbitrary, so the analytic solution to the Helmholtz equation cannot be found. In these circumstances, a numerical method should be developed to approximate solutions.

For numerically solving the Helmholtz equation, there are mainly finite difference methods [1] and finite element methods [2]. But in high dimensional Helmholtz problems, applying the mentioned methods has high computational costs and in irregular shaped domains getting good accuracy is very difficult and time consuming. Therefore in this work

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we employ the RBFs which are one of primary tools to interpolate multidimensional data. In the past decade, meshfree methods based on RBFs have received increased attention in approximating a solution for partial differential equations (PDEs) on regular and irregular domains. While spectral convergent property for these global numerical methods will be accessible if proper attention is paid to boundary conditions, they generally lead to large, ill-conditioned and full linear systems. RBF approximation is applied to solve option pricing problems in one and two spatial dimensions in [3], and numerical results show that RBF type method performs better than finite difference method. In [4], authors solved a forward Kolmogorov problem by using a meshfree method, and they got promising results. In [5] the RBFs meshless method is applied for the numerical solution of the nonlinear Benjamin-Bona-Mahony-Burgers equation on different domains. Also, they obtain a time semi-discretization method using forward finite difference scheme and a full discretization strategy by using the meshless method based on radial basis functions (RBFs) and Kansa's approach. In [6], authors first approximate the time fractional derivative of nonlinear Schrödinger equation by a scheme of order $2 - \alpha$ then use the Kansa approach to approximate the spatial derivatives. Also, RBF-based numerical strategies is employed to find a solution for the nonlinear sine-Gordon equation in [7].

In all of these mentioned global meshfree techniques, developed RBF collocation methods are leading to full linear systems, and have high computational costs basically when the number of dimensions increase. Localized RBF approximations such as the RBF partition of unity collocation method (RBF-PUM) and RBF-FD [8], [9] give an answer to deal with these issues. However, in the RBF-PUM finding the optimal number of patches in the domain of solution is a challenging problem and needs more computational considerations. The combination of meshfree and finite difference method known as RBF-FD method has been introduced and developed in [10]-[11]. Then, a generalization of the RBF-FD method that computes RBF-FD weights in finite-sized neighborhoods around the centers of RBF-FD stencils is developed in [12]. Moreover, in [13], we consider RBF-FD and Hermite finite difference methods for designing stencil weights and spatial discretization for time dependent PDEs of convection-diffusion-reaction type to show efficiency and applicability of this localized meshfree method.

In the present work, we consider RBF-FD and RBF-HFD methods for the approximation of the differential operator in Helmholtz problem. The aim of employing these methods is

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to improve the accuracy of the solution without increasing the stencil size, which is the usual way to increase the accuracy in the localized RBF methods. In the RBF-HFD scheme, the improvement in accuracy is obtained by using additional information from the PDE itself, rather than increasing the stencil size. Moreover, we show that the proposed methods lead to sparse matrices and we can control the computational costs and finally, numerical discussions confirm that the developed methods are efficient in complex geometries.

A. RBF-FD Methodology

To avoid mesh generation, in recent years meshless techniques have attracted the attention of researchers. In a meshless method a set of scattered nodes is used instead of meshing the domain of the problem. The technique of RBFs is one of the most recently developed meshless methods that has been used for different type of problems. The main advantages of RBF methods are as follow:

- No need for a mesh/triangulation.
- Simple implementation and dimension independence.
- No staircasing/polygonization for boundaries.
- Depending on chosen RBFs, high-order/spectral convergence can be achieved.
- Easy to implement derivatives and boundary conditions.

Firstly, in 1971 as a multidimensional scattered interpolation method, RBFs were developed by Hardy in modeling of the earth's gravitational field [14]. The application of RBFs based on collocation in a set of scattered nodes for the solution of PDEs was first proposed by Kansa [15]. Kansa's method was recently extended to solve various ordinary and partial differential equations, for instance see [16]-[17] and the references therein.

We consider a spatial domain $\Omega \subset \mathbb{R}^d$ and a set of distinct points $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$ in Ω. Also, let $\phi : \Omega \times \Omega \to \mathbb{R}$ be a kernel with the property $\phi(\mathbf{x}, \mathbf{y}) := \phi(\|\mathbf{x} - \mathbf{y}\|)$ for $\mathbf{x}, \mathbf{y} \in \Omega$, and $\|\cdot\|$ is the Euclidean norm. Kernels with this property known as radial functions. In Table I some globally supported RBFs are listed which are commonly employed in the literature. The positive constant ϵ appearing in RBFs is called the shape parameter which dictates the flatness of the radial basis function and also has a key role on the convergence rate of the approximations and the condition number of the coefficient matrices specifically for global methods. For more details about basic properties and types of radial basis functions, compactly and globally supported and also their wide applications in scattered date interpolations, the interested reader would be referred to recent works in this topic [18]-[19].

The RBF interpolant for a continuous target function $u : \Omega \to \mathbb{R}$ known at the nodes in $\mathbf{X}$ takes the form

$$\mathbb{I}_{\mathbf{X},u}(\mathbf{x}) = \sum_{j=1}^{N} \lambda_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{j=1}^{l} \nu_j p_j(\mathbf{x}), \qquad (3)$$

where $\|.\|$ is the Euclidean norm, and $\{p_j(\mathbf{x})\}_{j=1}^{l}$ denote basis of $\prod_{k-1}^{d}$, which is space of d-variate polynomials of total degree $\leq k-1$, where k is order of ϕ. If a polynomial space of

Name of function	Definition
Thin plate splines (TPS)	$(-1)^{k+1} r^{2k} \log(r)$
Gaussian (GA)	$\exp(-\epsilon^2 r^2)$
Invers multiquadrics (IMQ)	$\frac{1}{\sqrt{r^2 + \epsilon^2}}$
multiquadrics (MQ)	$\sqrt{r^2 + \epsilon^2}$
Conical splines	r^{2k+1}

degree $k-1$ is employed for $p_j(\mathbf{x})$, then $l = \begin{pmatrix} k+d-1 \\ d \end{pmatrix}$ see [20].

The interpolation coefficients $\{\lambda_j\}_{j=1}^{N}$ and $\{\nu_j\}_{j=1}^{l}$ are determined by imposing the following conditions

$$\mathbb{I}_{\mathbf{X},u}(\mathbf{x}_j) = u(\mathbf{x}_j), \quad j = 1, 2, \ldots, N$$

$$\sum_{j=1}^{N} \lambda_j p_k(\mathbf{x}_j) = 0, \quad k = 1, 2, \ldots, l.$$

This results in a symmetric system of linear equations

$$\begin{pmatrix} \mathbf{\Phi} & \mathbf{P} \\ \mathbf{P}^\top & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\nu} \end{pmatrix} = \begin{pmatrix} \mathbf{u} \\ \mathbf{0} \end{pmatrix} \qquad (4)$$

where

$$\mathbf{\Phi}_{i,j} = \phi(\|\mathbf{x}_i - \mathbf{x}_j\|), \quad i = 1, 2, ..., N, \quad j = 1, 2, ..., N$$

$$\mathbf{P}_{i,j} = p_j(\mathbf{x}_i), \quad i = 1, 2, ..., N, \quad j = 1, 2, ..., l$$

and $\boldsymbol{\lambda} = [\lambda_1, \lambda_2, \ldots, \lambda_N]^\top$, $\boldsymbol{\nu} = [\nu_1, \nu_2, \ldots, \nu_l]^\top$ and $\mathbf{u} = [u(\mathbf{x}_1), u(\mathbf{x}_2), \ldots, u(\mathbf{x}_N)]^\top$. When the points in $\mathbf{X}$ are chosen to be distinct and ϕ is a positive-definite radial kernel or order $k = 1$ conditionally positive-definite kernel on $\mathbb{R}^d$, the coefficient matrix of system (4) is guaranteed to be non-singular, see [21].

Now, let $\mathbf{X}_j = \{\mathbf{x}_1^{(j)}, \ldots, \mathbf{x}_n^{(j)}\} \subset \mathbf{X}$ be a subset containing $\mathbf{x}_j$ and its $n-1$ nearest neighboring points forming a stencil with $\mathbf{x}_j$ as center and $n \ll N$. The number of points n in each stencil can be either constant or vary with j. In the RBF-FD approach any linear differential operator $\mathcal{L}$ acting on $u(\mathbf{x})$ evaluated at $\mathbf{x}_j$, is approximated by a linear weighted combination of the function values of u at the points of $\mathbf{X}_j$,

$$\mathcal{L}u(\mathbf{x}_j) \approx \sum_{k=1}^{n} w_k^{(j)} u(\mathbf{x}_k^{(j)}). \qquad (5)$$

The RBF-FD weights, $w_k^{(j)}$, $k = 1, \ldots, n$, are found by enforcing that the approximation is exact within the space spanned by the RBFs $\{\phi(\|\mathbf{x} - \mathbf{x}_i^{(j)}\|)\}_{i=1}^{n}$, centered at the nodes $\mathbf{x}_i^{(j)}$, $i = 1, \ldots, n$ and solving the following linear system of equations

$$\begin{pmatrix} \mathbf{\Phi} & \mathbf{P} \\ \mathbf{P}^\top & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{w}^{(j)} \\ \boldsymbol{v}^{(j)} \end{pmatrix} =$$

$$\begin{pmatrix} (\mathcal{L}\phi(\|\mathbf{x}_j - \mathbf{x}_i^{(j)}\|)_{i=1}^{n})^\top \\ ((\mathcal{L}p_k(\mathbf{x}_j))_{k=1}^{l})^\top \end{pmatrix} \qquad (6)$$

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where $\boldsymbol{w}^{(j)} = [w_1^{(j)}, w_2^{(j)}, \ldots, w_n^{(j)}]^\top$ and $\boldsymbol{v}^{(j)} = [v_1^{(j)}, v_2^{(j)}, \ldots, v_l^{(j)}]^\top$. In the solution $w_1^{(j)}, w_2^{(j)}, \ldots, w_n^{(j)}$ are the weights applied to data at nodes $\mathbf{x}_i^{(j)}$ for $i = 1, 2, \ldots, n$. The rest of the solution vector $\boldsymbol{v}^{(j)}$ are discarded.

We have to solve this $(n + l) \times (n + l)$ linear system for each stencil center $\mathbf{x}_j$, $j = 1, \ldots, N$ to form the N rows of the sparse differentiation matrix with n non-zeros per row. In the context of time-dependent PDEs, the stencil weights remain constant for all time-steps when the nodes are stationary. With RBF-FD, the solutions are expected to converge algebraically and the system matrices are sparse and banded. For small shape parameter case with Gaussian RBF and RBF-QR, method can be used to generate the stencil weights in a stable way [22], [23].

Obviously, since $(n+l) \ll N$ the size of the linear systems (6) is much smaller than the size $N \times N$ of the linear system of a global RBF collocation method. A global RBF method to derive a differentiation matrix needs $O(N^3)$ operations, and results in a dense matrix. In the RBF-FD method we only need $O((n + l)^3)$ operations for each of the N stencils, so that the total cost of computing is $O((n + l)^3 N)$, without taking into account the cost of determining the stencil grids. For $n + l$ fixed with $(n + l) \ll N$, the total cost will be $O(N)$ for increasing N. The weights can be computed by inverting the local distance matrices $\boldsymbol{\Phi}$ of order $n \times n$ for each stencil. These distance matrices depend only on the distance of the grid points implying that for uniform grids we only need to compute the inverse of one local distance matrix. Further, the differentiation matrix for one stencil is independent from those for the other stencils. Hence their computation can be parallellized to increase the efficiency of RBF-FD method in high dimensional problems and adaptive algorithms.

B. RBF-HFD Methodology

In this section we review Hermite interpolation with RBFs proposed first by Wu [24], and in continue we derive RBF-HFD scheme by using Hermite interpolation with RBFs.

In the Hermite interpolation problem we find a function $\mathbb{I}_{\mathbf{X},u}(\mathbf{x})$ that interpolates u at the distinct nodes $\mathbf{x}_i, i = 1, \ldots, N$, and interpolates $\mathcal{L}u$ at $\tilde{\mathbf{x}}_j, j = 1, 2, \ldots, Q$ where $\mathcal{L}$ is a linear differential operator. To clarify the notation, assume that u is given at the nodes $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$ and $\mathcal{L}u$ is given at the nodes $\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \ldots, \tilde{\mathbf{x}}_Q$. Then Hermite interpolant with RBFs takes the form

$$\mathbb{I}_{\mathbf{X},u}(\mathbf{x}) = \sum_{j=1}^{N} \lambda_j \phi(\|\mathbf{x} - \mathbf{x}_j\|) + \sum_{j=1}^{Q} \vartheta_j \mathcal{L}_2 \phi(\|\mathbf{x} - \tilde{\mathbf{x}}_j\|)$$
$$+ \sum_{j=1}^{l} \nu_j p_j(\mathbf{x}), \quad (7)$$

and the interpolation coefficients $\{\lambda_j\}_{j=1}^{N}$, $\{\vartheta_j\}_{j=1}^{Q}$ and $\{\nu_j\}_{j=1}^{l}$ are determined by imposing the following conditions

$$\mathbb{I}_{\mathbf{X},u}(\mathbf{x}_j) = u(\mathbf{x}_j), \quad j = 1, 2, \ldots, N$$

$$\mathcal{L}(\mathbb{I}_{\mathbf{X},u})(\tilde{\mathbf{x}}_j) = \mathcal{L}(u(\tilde{\mathbf{x}}_j)), \quad j = 1, 2, \ldots, Q$$

$$\sum_{j=1}^{N} \lambda_j p_k(\mathbf{x}_j) = 0, \quad k = 1, 2, \ldots, l.$$

This results in a symmetric system of linear equations

$$\begin{pmatrix} \boldsymbol{\Phi} & \boldsymbol{\Psi}_2 & \mathbf{P} \\ \boldsymbol{\Psi}_1 & \boldsymbol{\Psi}_{12} & 0 \\ \mathbf{P}^\top & 0^\top & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\vartheta} \\ \boldsymbol{\nu} \end{pmatrix} = \begin{pmatrix} \mathbf{u} \\ \mathcal{L}u \\ 0 \end{pmatrix} \quad (8)$$

where $\boldsymbol{\Phi}, \mathbf{P}, \boldsymbol{\lambda}$ and $\boldsymbol{\nu}$ were defined before and

$$(\boldsymbol{\Psi}_2)_{i,j} = \mathcal{L}_2 \phi(\|\mathbf{x}_i - \tilde{\mathbf{x}}_j\|), \quad i = 1, 2, \ldots, N, \quad j = 1, 2, \ldots, Q$$

$$(\boldsymbol{\Psi}_1)_{i,j} = \mathcal{L}_1 \phi(\|\tilde{\mathbf{x}}_i - \mathbf{x}_j\|), \quad i = 1, 2, \ldots, Q, \quad j = 1, 2, \ldots, N$$

$$(\boldsymbol{\Psi}_{12})_{i,j} = \mathcal{L}_1 \mathcal{L}_2 \phi(\|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|), \quad i, j = 1, 2, \ldots, Q,$$

and $\boldsymbol{\vartheta} = [\vartheta_1, \vartheta_2, \ldots, \vartheta_Q]^\top$ and $\mathcal{L}u = [\mathcal{L}u(\tilde{\mathbf{x}}_1), \mathcal{L}u(\tilde{\mathbf{x}}_2), \ldots, \mathcal{L}u(\tilde{\mathbf{x}}_Q)]^\top$. Also, in the above definitions of matrices elements $\mathcal{L}_1$ and $\mathcal{L}_2$ stand that $\mathcal{L}$ is applied to ϕ with respect to its first and second arguments, respectively. If radial basis function ϕ is a positive definite or conditionally positive definite of order-1, then the linear system (8) is nonsingular [24], [25].

The main goal of using RBF-HFD is to increase the accuracy of the approximation (5) without increasing the stencil size. Now for deriving RBF-HFD scheme, let $\mathbf{X}_j = \{\mathbf{x}_1^{(j)}, \ldots, \mathbf{x}_n^{(j)}\} \subset \mathbf{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ be a subset containing $\mathbf{x}_j$ and its $n - 1$ nearest neighboring points forming a stencil with $\mathbf{x}_j$ as center and $n \ll N$. In the RBF-HFD approach any linear differential operator $\mathcal{D}$ acting on $u(\mathbf{x})$ evaluated at $\mathbf{x}_j$, is approximated by a linear weighted combination of the function values of u at the points of $\mathbf{X}_j$ and $\mathcal{D}u$ at the points of $\tilde{\mathbf{X}}_j = \{\tilde{\mathbf{x}}_1^{(j)}, \ldots, \tilde{\mathbf{x}}_q^{(j)}\}$ for $q \ll Q$,

$$\mathcal{D}u(\mathbf{x}_j) \approx \sum_{k=1}^{n} w_k^{(j)} u(\mathbf{x}_k^{(j)}) + \sum_{k=1}^{q} \tilde{w}_k^{(j)} \mathcal{L}u(\mathbf{x}_k^{(j)}). \quad (9)$$

The RBF-HFD weights, $w_k^{(j)}$ for $k = 1, \ldots, n$ and $\tilde{w}_k^{(j)}$ for $k = 1, \ldots, q$ are found by enforcing that the approximation is exact within the space spanned by the RBFs $\{\phi(\|\mathbf{x} - \mathbf{x}_i^{(j)}\|)\}_{i=1}^{n}$ centered at the nodes $\mathbf{x}_i^{(j)}$, $i = 1, \ldots, n$ and $\{\mathcal{L}_2 \phi(\|\mathbf{x} - \tilde{\mathbf{x}}_i^{(j)}\|)\}_{i=1}^{q}$ centered at the nodes $\tilde{\mathbf{x}}_i^{(j)}$, $i = 1, \ldots, q$ and $\{p_j(\mathbf{x})\}_{j=1}^{l}$. This can be written as the following linear system

$$\begin{pmatrix} \boldsymbol{\Phi} & \boldsymbol{\Psi}_2 & \mathbf{P} \\ \boldsymbol{\Psi}_1 & \boldsymbol{\Psi}_{12} & 0 \\ \mathbf{P}^\top & 0^\top & 0 \end{pmatrix} \begin{pmatrix} \mathbf{w}^{(j)} \\ \widetilde{\mathbf{w}}^{(j)} \\ \mathbf{v}^{(j)} \end{pmatrix} =$$

$$\begin{pmatrix} (\mathcal{D}_1 \phi(\|\mathbf{x}_j - \mathbf{x}_i^{(j)}\|)_{i=1}^{n})^\top \\ (\mathcal{D}_1 \mathcal{L}_2 \phi(\|\mathbf{x}_j - \mathbf{x}_i^{(j)}\|)_{i=1}^{q})^\top \\ ((\mathcal{D}p_k(\mathbf{x}_j))_{k=1}^{l})^\top \end{pmatrix} \quad (10)$$

where $\mathcal{D}_1$ stands that $\mathcal{D}$ is applied to ϕ with respect to its first argument. Note that the rest of the solution vector $\mathbf{v}^{(j)}$ are discarded.

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C. Numerical Results

In this section, we present a numerical example to compute the solution of fractional convection-diffusion-reaction problem using the RBF-FD and RBF-HFD methods and show efficiency and applicability of presented numerical method. We are using MATLAB with a 3.6 GHz Corei3 processor to do all computations. In our computation, we employ the multiquadric $\phi(r) = \sqrt{\varepsilon^2 + r^2}$ as radial basis function. To illustrate the accuracy of method, we compute the following error norms:

$$L_\infty = \max_{1 \le j \le N} \left| u^{exact}(\mathbf{x}_j) - u^{numerical}(\mathbf{x}_j) \right|,$$

$$RMS = \sqrt{\frac{1}{N} \sum_{j=1}^{N} \left(u^{exact}(\mathbf{x}_j) - u^{numerical}(\mathbf{x}_j) \right)^2},$$

where N is the number of the test points, $u^{numerical}(\mathbf{x}_j)$ and $u^{exact}(\mathbf{x}_j)$ denote the numerical and analytical solutions at the jth test point, respectively. The errors are evaluated over 2046 test points which are perturbed randomly in the direction of the boundary.

Example 1. Consider the following three-dimensional Helmholtz problem

$$\nabla^2 u(\mathbf{x}) + u(\mathbf{x}) = 0, \qquad \mathbf{x} \in \Omega.$$

Boundary conditions at the surface are chosen based on the exact solution

$$u(x, y, z) = \cos(x) + \sin(y) + \sin(z),$$

where Ω is a solid domain bounded by the surface

$$x^2 + y^2 + z^2 - \sin(2x)^2 \sin(2y)^2 \sin(2z)^2 = 1. \qquad (11)$$

Fig. 1 shows the solid domain bounded by the surface equation (11). The L_∞ and RMS errors and CPU times are reported in Table 1. Comparison between the presented methods shows that the RBF-HFD method is more accurate.
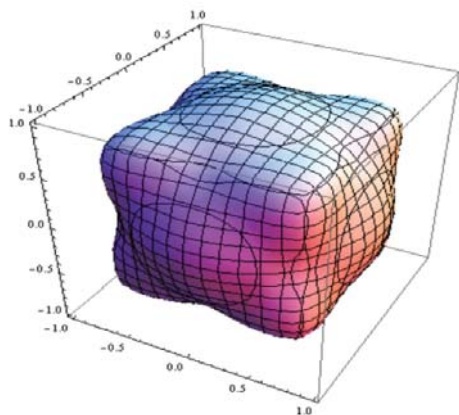

Fig. 1 The solid domain bounded by the surface equation (11)

TABLE II
COMPARISON OF ERRORS FOR EXAMPLE 1

Methods	n	q	L_∞	RMS	CPU time(s)
RBF-FD	27	0	8.3774e-04	3.0722e-04	4.75
RBF-FD	40	0	3.7623e-05	1.4537e-05	5.39
RBF-HFD	27	26	5.5677e-05	1.9210e-05	5.81
RBF-HFD	40	39	2.4231e-06	3.8299e-07	7.25

II. CONCLUSION

For approximation of differential operator in this study we employ two localized meshfree techniques known as RBF-FD and RBF-HFD schemes which result in sparse matrices as well as the standard FD method, but with the added advantage that the RBF method can naturally handle irregular geometries, we compared RBF-FD and RBF-HFD methods in irregular domain, and numerical results show the efficiency and performance of both RBF-FD and RBF-HFD methods, but RBF-HFD is more accurate than RBF-FD in irregular geometry of solution domain.

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