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An improved subspace selection algorithm for meshless collocation methods

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SUMMARY

Choosing data points is a common problem for researchers who employ various meshless methods for solving partial differential equations. On one hand, high accuracy is always desired; on the other, ill-conditioning problems of the resultant matrices, that may lead to unstable algorithms, prevent some researchers from using meshless methods. For example, the optimal placements of source points in the method of fundamental solutions, or of the centers in the radial basis functions method are always unclear. Intuitively, such optimal locations will depend on many factors: the partial differential equations, the domain, the trial basis used (i.e. the employed method itself), the computational precisions, some user defined parameters, and so on. Such complexity makes the hope of having an optimal centers placement unpromising. In this paper, we provide a data-dependent algorithm that adaptively selects centers based on all the other variables. Copyright © 2000 John Wiley & Sons, Ltd.

1. Introduction

Many successful applications of meshless methods have recently been studied in science and engineering; particular examples include the convection-diffusion problems [26], elliptic problems [6], near singular Poisson problems [7], Dual reciprocity method [5, 12], biharmonic equation [23], Stokes problems [41], potential problems [40], non-linear thermal explosions [4], eigenfrequencies of plate vibrations [42], financial mathematics [14, 31], etc. Many other successful applications based on either the method of fundamental solutions (MFS) or the radial basis function (RBF) method can be found in different Mathematics, Physics and Engineering journals [8, 9, 13, 16, 18, 19, 26, 32]. Instead of working on a specific applications, we propose a new algorithm that allows researchers to use these meshless methods without worrying the ill-conditioning problem.

For the MFS, it is shown [11] that the accuracy (for compatible problems) will depend on the placement of source points. It is suggested [1] that placing the source points equispaced

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in the normal direction from the boundary can improve the accuracy of MFS. Similarly, the conditioning and accuracy of the RBF method greatly depends on the user defined radial basis centers and the so-called shape parameter c. Most commonly used RBFs $\Phi(r)$ can be scaled by a simple transform $r \leftarrow r/c$ where c is referred as the shape parameter. Besides of the separating distance h of the centers, the accuracy of RBF methods is severely influenced by the shape parameter c. As the shape parameter c gets large, the RBFs become flat and consequently the resultant system of equations for the expansion coefficients becomes badly conditioned. The trade-off for this increased accuracy and ill-conditioning of the associated linear systems can be explained by the "uncertainty relation" given by Schaback [34, 35, 36]. Our goal, instead of finding optimal value, is to provide a stable procedure as independent as possible of the user-defined parameter. The search for best shape parameter is still an open problem. In [39], the role of c to the accuracy of the RBF method is examined. An algorithm for selecting a good value for the parameter c in the radial basis function interpolation can be found in [33]. Recently, Huang et al. [17] provides some numerical procedures for searching such parameter.

On the other hand, good distributions of RBF centers do not get as much attentions mainly due to the high degree of freedom of the underlying problem. Our previous work [29] provides an adaptive algorithm to select RBF centers from a large set of candidates. In this paper, we propose an improved algorithm (over the one in [29]) that picks "good" RBF centers by introducing a new selection criterium. Our discussion will focus on the unsymmetric RBF collocation method, also known as the Kansa's method; however, the method in this paper can be directly applied to the MFS for source points selection.

First of all, we give a brief introduction to the unsymmetric RBF collocation method and introduce some notations for the rest of the work. Consider the boundary value problems of the form

$$\begin{array}{rcll} \mathcal{L}u & = & f & \text{in } \Omega \subset \mathbb{R}^d, \\ \mathcal{B}u & = & g & \text{on } \partial\Omega, \end{array} \tag{1}$$

where d denotes the spatial dimension, $\partial\Omega$ denotes the boundary of the domain Ω, $\mathcal{L}$ is an interior differential operator and $\mathcal{B}$ is an operator that specifies the boundary conditions of Dirichlet, Neumann or mixed type. Both f, $g : \mathbb{R}^d \to \mathbb{R}$ are given smooth functions.

In the unsymmetric RBF collocation method, the unknown solution u of (1) is approximated by a linear combination of RBFs in the form of

$$u(x) \approx u_N(x) = \sum_{k=1}^{N} \lambda_k \, \Phi(\|x - \xi_k\|), \tag{2}$$

where $\Xi_N = \{\xi_k\}_{k=1}^N$ be an indexed set of the N RBF centers. In the original Kansa's formulation [20, 21], the set of centers and collocation points are identical. In the present paper, the link between the two sets of points is decoupled as motivated by the solvability theory in [29]. In particular, one shall take $N \geq M$ to ensure solvability.

Using the collocation method to ensure that the approximation $u_N(x)$ satisfies (1) at a set of M collocation points X_M, we obtain a numerical approximation of u. If we assume the set of collocation points X_M is indexed and is arranged in such a way that the first m_I points and the last m_B points are in Ω and on $\partial\Omega$, respectively. To solve for the N unknown coefficients $\lambda = [\lambda_1, \ldots, \lambda_N]^T$ in (2), we need to solve the following N linearly independent equations

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$$\begin{aligned} \sum_{k=1}^{N} \lambda_k \mathcal{L}\Phi(\|x_i - \xi_k\|) &= f(x_i) \quad \text{for } i = 1, \ldots, m_I, \\ \sum_{k=1}^{N} \lambda_k \mathcal{B}\Phi(\|x_i - \xi_k\|) &= g(x_i) \quad \text{for } i = m_I + 1, \ldots, M. \end{aligned} \tag{3}$$

Rewriting (3) in matrix form, we have the *resultant system* given by

$$\begin{bmatrix} \Psi_{\mathcal{L}} \\ \Psi_{\mathcal{B}} \end{bmatrix} \lambda = \begin{bmatrix} f \\ g \end{bmatrix}, \qquad \text{or} \qquad A\lambda = b, \tag{4}$$

where $f \in \mathbb{R}^{m_I}$, $g \in \mathbb{R}^{m_B}$, $\Psi_{\mathcal{L}} \in \mathbb{R}^{m_I \times N}$, $\Psi_{\mathcal{B}} \in \mathbb{R}^{m_B \times N}$ with entries

$$\begin{array}{rcll} [f]_i & = & f(x_i), & \text{for } i = 1, \ldots, m_I, \\ [g]_i & = & g(x_i), & \text{for } i = 1, \ldots, m_B, \\ [\Psi_{\mathcal{L}}]_{ik} & = & \mathcal{L}\Phi(\|x_i - \xi_k\|), & \text{for } i = 1, \ldots, m_I,\ k = 1, \ldots, N, \\ [\Psi_{\mathcal{B}}]_{ik} & = & \mathcal{B}\Phi(\|x_i - \xi_k\|), & \text{for } i = m_I + 1, \ldots, M,\ k = 1, \ldots, N. \end{array} \tag{5}$$

The matrix given by (4)–(5) is generally unsymmetric and full. Note that the problem of ill-conditioning is not taken into account yet.

The algorithm proposed in [29] and which is also used in this work is based on the so-called greedy technique. The basic idea of this technique is to make a sequential selection of points based on the largest entry-wise residuals. In [38], Schaback and Wendland employ the greedy techniques for solving large interpolation systems arising form compactly-supported RBF. Under the symmetric formulation, applying the greedy technique selects both the RBF centers and collocation points. Such idea has been brought towards the symmetric RBF collocation method, see [15]. When we moved away from the symmetric setting towards the unsymmetric one, the immediate problem is the decoupling of the RBF centers and the collocation points. Namely, picking a collocation point by studying the residual vector provides no information for the problem of RBF center selection.

In [29], we propose the first greedy version of adaptive algorithm for unsymmetric and global RBF collocation system. The RBF centers are selected based on the determinant function and ensure local solvability. With a fast formula, such selection can be done efficiently without the evaluation or storage of the full matrix. Moreover, the algorithm is data-dependent in a way that the right-hand vector is taken into account. More numerical results can be found in [25].

The key advance of this work is the introduction of another criterium for RBF centers selection. The current paper is outlined as follows: an adaptive RBF centers selection algorithm is proposed based on the primal-dual formulation of the minimum-norm solution to an overdetermined system. The selection relies on the greedy technique that is overviewed in the next section. The proposed algorithm is introduced in Section 2.2. The implementation and cost of the proposed algorithm is also studied. Furthermore, some geometric interpretations of the greedy technique are provided. In Section 3, some numerical results are presented to show that the newly proposed algorithm outperforms the previous one. Finally, the paper is concluded in Section 4

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2. Adaptive trial space selection

To solve the ill-conditioned unsymmetric collocation systems, the rounding error will eventually have great impact on the accuracy. We will circumvent the problem by adaptively selecting the *best* trial space for approximation.

Consider any underdetermined system $A \in \mathbb{R}^{M\times N}$ and $b \in \mathbb{R}^M$ with $M \le N$. Then, the minimum norm solution can be obtained through the following constrained minimization problem:

$$\begin{cases} \text{minimize} & \frac{1}{2}\lambda^T I\lambda, \\ \text{subject to} & A\lambda - b = 0. \end{cases} \tag{6}$$

Using the method of Lagrange multipliers, the primal-dual formulation of Problem (6) can be rewritten as block form

$$\mathcal{A}\begin{bmatrix} \lambda \\ \nu \end{bmatrix} := \begin{bmatrix} I & A^T \\ A & 0 \end{bmatrix}\begin{bmatrix} \lambda \\ \nu \end{bmatrix} = \begin{bmatrix} 0 \\ b \end{bmatrix}, \tag{7}$$

where $\nu \in \mathbb{R}^M$ is the vector of Lagrange multipliers, $I_N \in \mathbb{R}^{N\times N}$ is the identity matrix and $0 \in \mathbb{R}^{M\times M}$ is the zero matrix. In the next section, an adaptive algorithm for selecting RBF centers (as well as collocation points) is built upon (7).

2.1. Adaptive algorithm

In this section, different submatrices of the collocation matrix A and b are needed. Since A is completely determined by the collocation points and the RBF centers, we denote submatrices of A by $A(\,\cdot\,,\,\cdot\,) : (\mathbb{R}^d)^m \times (\mathbb{R}^d)^n \to \mathbb{R}^{m\times n}$ as a matrix function taking sets of collocation points and sets of RBF centers, respectively, as the first and second input arguments. Similar, the right-hand vector $b(\,\cdot\,) : (\mathbb{R}^d)^m \to \mathbb{R}^m$ can be treated as a vector function that can be specified by the collocations points. For example, $A = A(X_M, \Xi_N) \in \mathbb{R}^{M\times N}$ and $b = b(X_M) \in \mathbb{R}^M$ are, respectively, the original full matrix and the right-hand vector in (4).

We propose an algorithm to build a new indexed sets, denoted by $X_{(k)} = \{x_{(1)}, \ldots, x_{(k)}\}$ and $\Xi_{(k)} = \{\xi_{(1)}, \ldots, \xi_{(k)}\}$ $(k = 1, \ldots, M)$ for the collocation points and RBF centers respectively, such that the chosen ones are listed earlier in the lists. Suppose, after k iterations, our algorithm selected a set of k collocation points $X_{(k)} \subset X_M$ and a set k RBF centers $\Xi_{(k)} \subset \Xi_N$, respectively. These sets of points define a subproblem to the original one:

$$\begin{cases} A_{(k)}\check{\lambda}^{(k)} = & \check{b}^{(k)}, \\ A_{(k)}^T\check{\nu}^{(k)} = & -\check{\lambda}^{(k)}, \end{cases} \tag{8}$$

where $A_{(k)} = A(X_{(k)}, \Xi_{(k)}) \in \mathbb{R}^{k\times k}$ is a square submatrix of the full matrix A and $\check{b}^{(k)} = b(X_{(k)}) \in \mathbb{R}^k$. After solving (8) for $\check{\lambda}^{(k)} \in \mathbb{R}^k$, let $\lambda^{(k)} \in \mathbb{R}^N$ be the extension of $\check{\lambda}^{(k)}$ by patching zeros into entries associated with the non-selected RBF centers. Similar, $\check{\nu}^{(k)} \in \mathbb{R}^k$ can be extended to $\nu^{(k)} \in \mathbb{R}^N$.

The primal PDE residual, with respect to the intermediate solution $\lambda^{(k)}$, can be computed by

$$r^{(k)} = A\lambda^{(k)} - b = A(X_M, \Xi_{(k)})\check{\lambda}^{(k)} - b. \tag{9}$$

From (7), one can investigate how well the Lagrange conditions,

$$\nabla_\lambda\left(\frac{1}{2}\lambda^T I\lambda + \nu(A\lambda - b)\right) = 0,$$

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are being satisfied by looking at the dual PDE residual

$$q^{(k)} = \lambda^{(k)} + A^T \nu^{(k)} = \lambda^{(k)} + [A(X_{(k)}, \Xi_N)]^T \check{\nu}^{(k)}. \tag{10}$$

The $(k+1)^{\text{st}}$ collocation point $x_{(k+1)}$ and the RBF center $\xi_{(k+1)}$ can be selected from (9) and (10), respectively, using the *greedy* technique. We pick from the set of collocation points X_M a collocation point $x_{(k+1)}$ such that the corresponding entry in the primal residual $r^{(k)}$ is the largest in absolute value. Similarly, the new RBF center $\xi_{(k+1)}$ is selected from all candidates in Ξ_N such that the dual residual $q^{(k)}$ is the largest in absolute value among all others. The iterations should stop if either residual (9)–(10) is smaller than some tolerance or if severe ill-conditioning in (8) is detected.

2.2. Implementation and cost

The proposed adaptive greedy method aims for huge but finite Kansa's resultant systems that is severely ill-conditioned. The matrix-free feature of the proposed algorithm means that the *a priori* evaluation and storage of the full matrix is unnecessary. Moreover, it is different from the standard elimination techniques with pivoting because it takes the right-hand side into account. If applied to some ill-conditioned linear systems, the proposed method will terminate earlier since fewer RBF centers are needed to make the linear solver breakdown.

Startup is done by finding some collocation points $x_{(1)} \in X_M$ from the primal residual $r^{(1)} = b \neq 0$ and an arbitrary RBF center $\xi_{(1)}$. For all numerical demonstrations in this work, we take $\xi_{(1)}$ such that $A(\{x_1\}, \cdot)$ is maximized. This ensures $A_{(1)} \in \mathbb{R}^{1\times 1}$ is nonzero and hence invertible. For some user defined integers $k_{max} \leq M \leq N$, the algorithm then iterates on $k = 2, 3, \ldots, k_{max}$ as follows:

1. Compute and store all entries of the row $A(\{x_{(k-1)}\}, \Xi_N)$ corresponding to the previously selected collocation point $x_{(k-1)}$; this takes $\mathcal{O}(M)$ operations.
2. Compute and store all entries of the column $A(X_M, \{\xi_{(k-1)}\})$ corresponding to the previously selected RBF center $\xi_{(k-1)}$; this takes $\mathcal{O}(N)$ operations.
3. Solve the subproblem (8) for $\check{\lambda}^{(k)}$ and $\check{\nu}^{(k)}$ using some direct methods; this takes $\mathcal{O}(k^3)$ operations. Note that the submatrix $A_{(k)}$ can be extracted from the stored rows (or columns) of A.
   - STOP if ill-conditioning problem is detected[†], or if $k = K$.
4. Compute the primal residual $r^{(k)}$ and dual residual $q^{(k)}$ as in (9) and (10) using $\check{\lambda}^{(k)}$ and $\check{\nu}^{(k)}$ with the computed columns and rows of A, respectively. These take $\mathcal{O}(kN)$ and $\mathcal{O}(kM)$, respectively. Note that the extended vectors $\lambda^{(k)}$ and $\nu^{(k)}$ are not needed.
5. Select a new RBF center $\xi_{(k)}$ by finding the entry in $q^{(k)}$ with maximum magnitude.
6. Select a new collocation point $x_{(k)}$ by finding the entry in $r^{(k)}$ with maximum magnitude.
   - STOP if the computed values in $r^{(k)}$ are smaller than some tolerance.
7. Repeat the iteration for $k + 1$.

[†]In our Matlab implementation, the algorithm will terminate if the *BACKSLASH* (or *MLDIVIDE*) function call shows the "*Warning: Matrix is close to singular or badly scaled.*"

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Within the k^{th} iteration , the previously proposed algorithm in [29] requires the solutions of $N+1$ systems of size $k \times k$ such that, in Step 6, a new collocation point is selected to provide a new $(k+1) \times (k+1)$ system with determinant closest to 1. The proposed primal-dual criteria requires the solutions of two $k \times k$ subsystems only.

Suppose the above iteration terminates at step $k_t \leq k_{max} \leq M$. The total work of the proposed adaptive greedy method is $\mathcal{O}(k_t^2(k_t^2 + M + N))$ and the total storage requirement is $\mathcal{O}(k_t(M+N))$ for the selected rows and columns of A. The computational cost can be further reduced to $\mathcal{O}(k_t^2(k_t + M + N))$ if a matrix inverse update formula, as in [29], is employed in Step 3. Figure 1 schematic illustration of the selected RBF centers.

The proposed algorithm is attractive in solving PDE with smooth solution in higher dimensions. In such cases, good results can be expected from using a large shape parameter c. Moreover, the final iteration count k_t is expected to be small as rather small number of basis is needed for good approximation. Here, the proposed algorithm provides good confidence for one to employ a large c in the formulation.

Suppose one wants to solve a PDE with the original Kansa's method with N nodes; this costs $\mathcal{O}(N^3)$. Now, if the proposed method is employed with N collocation points and double the number of trial RBF centers, and we stop at the $k_{max} = N$ steps at maximum, then the computational complexity is less than $\mathcal{O}(N^2(N + N + 2N) = \mathcal{O}(N^3)$. Note that, depending on the conditioning of the underneath matrix, it may not be possible to reach N iterations. Using the proposed method is more expensive but in the same order of complexity as using the original Kansa's method. The extra cost is paid off in two ways: the selected RBF centers are now optimized, and, we have a safeguard from getting unless numerical solution (when c is chosen to be too large).

The following theorem guarantees solvability at each iteration.

Theorem 1. *If $r^{(k)}, q^{(k)} \neq 0$ so that the selections of new collocation point $x_{(k+1)}$ and RBF center $\xi_{(k+1)}$ are possible, and if the square submatrix $A_{(k)} = A(x_{(k)}, \xi_{(k)})$ in the previous step is nonsingular, then $A_{(k+1)} = A(x_{(k+1)}, \xi_{(k+1)})$ is also nonsingular.*

Proof. By construction, the $(k+1) \times (k+1)$ matrix $A_{(k+1)}$ has the form

$$A_{(k+1)} = \begin{bmatrix} A_{(k)} & v \\ u^T & w \end{bmatrix} = \begin{bmatrix} A_{(k)} & 0 \\ 0^T & 1 \end{bmatrix} \begin{bmatrix} I_k & A_{(k)}^{-1}v \\ u^T & w \end{bmatrix}, \text{ where } u, v \in \mathbb{R}^k,\ w \in \mathbb{R}.$$

It is straightforward to show that $\det(A_{(k+1)}) = (w - u^T A_{(k)}^{-1} v) \det(A_{(k)})$.

It remains to show that $w - u^T A_{(k)}^{-1} v$ is nonzero. Consider the matrix system $A_{(k+1)} \check{\lambda}^{(k+1)} = b^{(k+1)}$ in block form

$$\underbrace{\begin{bmatrix} A_{(k)} & v \\ u^T & w \end{bmatrix}}_{A_{(k+1)}} \underbrace{\begin{bmatrix} y \\ \eta \end{bmatrix}}_{\check{\lambda}^{(k+1)}} = \underbrace{\begin{bmatrix} b^{(k)} \\ \beta \end{bmatrix}}_{b^{(k+1)}}, \quad y \in \mathbb{R}^k,\ \eta, \beta \in \mathbb{R}. \tag{11}$$

From the first equation and the fact that $b^{(k)} = A_{(k)} \check{\lambda}^{(k)}$, we obtain $y = \check{\lambda}^{(k)} - \eta A_{(k)}^{-1} v$. Put this to the second equation in (11) to obtain

$$-\eta(w - u^T A_{(k)}^{-1} v) = u^T \check{\lambda}^{(k)} - \beta = \|r^{(k)}\|_\infty \neq 0.$$

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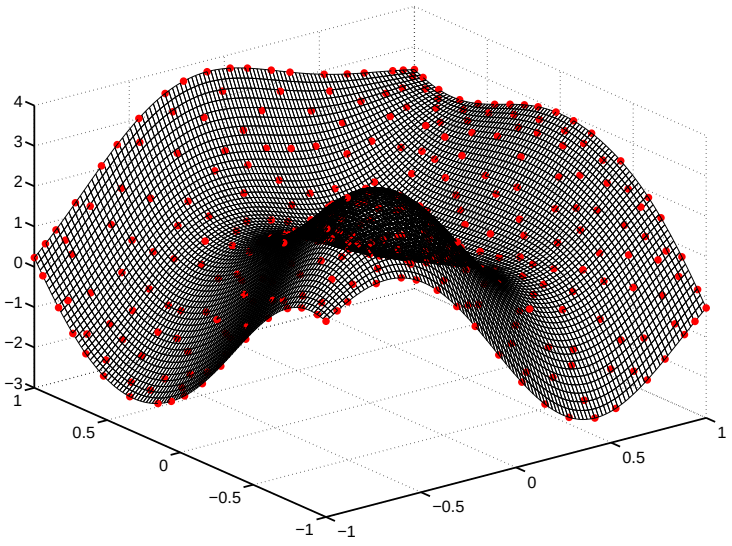

Figure 1. Schematic illustration of the selected RBF centers

Hence, $\det(A_{(k+1)})$ is nonzero and $A_{(k+1)}$ is nonsingular. Moreover, we also show that the last entry of $\check{\lambda}^{(k+1)}$ will always be nonzero. In other words, the newly introduced RBF center will always be used. □

2.3. Determining the unknown coefficients

After termination at step k_t, the end result of the greedy algorithm in Section 2.2 is two set of points: k_t collocation points in $X_{(k_t)} = \{x_{(1)}, \ldots, x_{(k_t)}\}$ and k_t RBF centers in $\Xi_{(k_t)} = \{\xi_{(1)}, \ldots, \xi_{(k_t)}\}$.

The selected RBF centers are used to define a trial space and the approximate solution are expanded as in (2). Motivated by the convergent theory [37], unknown coefficients are chosen not only based on the selected k_t conditions but on a *large* set of collocation points. If we simply take the original set X_M as such large set, the final step is to solve an $M \times k_t$ overdetermined system, using the least-squares approach,

$$A(X_M, \Xi_{(k_t)})\lambda_{k_t} = b,$$

for the approximate solution λ_{k_t} to $A\lambda = b$ which requires $\mathcal{O}(k_t^2 M)$ operations.

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2.4. Greedy techniques revisit

Following the geometric interpretation of the row projection method [2] for saddle point systems, we represent the Kansa's matrix by its row as

$$A = \begin{bmatrix} g_1^T \\ \vdots \\ g_m^T \end{bmatrix}.$$

Let the square bracket $[\,\cdot\,]_i$ denote the i^{th} entry of a vector; the right-hand vector has entries $b = ([\,b\,]_1, \ldots, [\,b\,]_M)^T$. Then, the M equations in (4), that is the M collocation conditions, gives M hyperplanes in $\mathbb{R}^N$. These hyperplanes can be explicitly written down as

$$\mathcal{H}_i := \left\{ z \in \mathbb{R}^N \ : \ g_i^T z = [\,b\,]_i \right\} \ \text{ for } \ i = 1, \ldots, M.$$

Let $\mathcal{G} := \bigcap \mathcal{H}_i$ be the subset of $\mathbb{R}^N$ that is the intersection of all M hyperplanes. We can formulate Problem (6) as seeking $\lambda \in \mathcal{G}$ with minimum norm. The proposed adaptive criteria for collocation points and RBF centers can be interpreted geometrically by the following theorems.

Theorem 2. *The i-th entry of the greedy primal residual $r^{(k)} \in \mathbb{R}^M$ is a scaled distance between the k-th iterative solution $\lambda^{(k)}$ and the i-th hyperplane.*

Proof. Consider any hyperplane $\mathcal{H}_i$ $(i = 1, \ldots, M)$ and observe that $\lambda^{(k)} \in \mathbb{R}^N$ can be uniquely decomposed, by orthogonal projections, into $\lambda^{(k)} = \mathcal{P}_{\mathcal{H}_i} \lambda^{(\|)} + \mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(\|)}$ where $\mathcal{P}_{\mathcal{H}_i} \lambda^{(k)} \in \mathcal{H}_i$ and $\mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} \in \mathcal{H}_i^\perp$. In this proof, $\|\cdot\| = \|\cdot\|_2$. Since $\mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)}$ is pointing in the normal direction of the hyperplane $\mathcal{H}_i$, we can represent $\mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} = \left\| \mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} \right\| \hat{n}_i$ where $\hat{n}_i = g_i / \|g_i\|$. Hence, we have

$$\begin{aligned} \lambda^{(k)} &= \mathcal{P}_{\mathcal{H}_i} \lambda^{(k)} + \mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} \\ g_i^T \lambda^{(k)} &= g_i^T \mathcal{P}_{\mathcal{H}_i} \lambda^{(k)} + g_i^T \mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} \\ g_i^T \lambda^{(k)} &= [\,b\,]_i + \left\| \mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} \right\| g_i^T \hat{n}_i \\ \left\| \mathcal{P}_{\mathcal{H}_i^\perp} \lambda^{(k)} \right\| &= (g_i^T \lambda^{(k)} - b_i) / \|g_i\|. \end{aligned}$$

Note that $g_i^T \lambda^{(k)} - [\,b\,]_i = [r^{(k)}]_i$ is the i-th entry of the greedy primal residual $r^{(k)}$. The assertion is proven. □

Theorem 3. *The norm of the greedy dual residual $q^{(k)}$ is larger than the distance between the k-th iterative solution $\lambda^{(k)}$ and the subspace $\mathcal{G}^\perp$ with respect to the same norm. In particular, the proposed algorithm takes $\|q^{(k)}\|_\infty$ as the RBF center selection criteria.*

Proof. Note that $\mathcal{G}$ is parallel to $\operatorname{Nul} A$. Clearly, $-A^T \nu^{(k)} \in \mathcal{G}^\perp = \operatorname{Row} A$. Hence, $\operatorname{dist}(\lambda^{(k)}, \operatorname{Row} A) \le \operatorname{dist}(\lambda^{(k)}, -A^T \nu^{(k)}) = \|q^{(k)}\|$. □

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3. Numerical demonstrations

In this section, some numerical examples are shown to demonstrate the stability and convergent behaviours of our proposed algorithms, *new-Greedy*, in double–precision and to compare with the accuracy of the previously proposed method, abbreviated as *old-Greedy*. In all examples, we have used the multiquadric kernel

$$\Phi_c(r) = \sqrt{c^2 + r^2},$$

in (2) where $r \in \mathbb{R}$ and $c > 0$. As a test problem, we solve the Poisson equation with the Dirichlet boundary conditions, i.e.

$$\begin{aligned} \triangle u(x) &= f(x) \quad \text{for } x \in \Omega \subset \mathbb{R}^d, \\ u(x) &= g(x) \quad \text{for } x \in \partial\Omega. \end{aligned} \tag{12}$$

on the unit square $\Omega = [-1, 1]^d$ $(d = 2, 3)$ for easy reproduction of the presented numerical results. The power of meshless method, still, is its capability in solving problems in complicated geometries.

3.1. Example 1

The functions f and g in (12) are generated by the `peaks` function (as the exact solution, see Figure 1) given by

$$u^* = 3(1-x)^2 e^{-x^2-(y+1)^2} - 10(\frac{x}{5} - x^3 - y^5)e^{-x^2-y^2} - \frac{1}{3}e^{-(x+1)^2-y^2}.$$

The numerical results in [29, 30] suggest the improvement of accuracy if one allows the greedy algorithm to select RBF centers outside Ω. For the sake of easy comparison, we employ the setting in the original Kansa's method. We take $X_M \equiv \Xi_N$ and, moreover, the points are regularly spaced in Ω with separating distance h. That is

$$M = N = (h^{-1} + 1)^2.$$

Having randomly distributed points, even with very small separating distance, will not dramatically affect the performance of the proposed method. All errors of the approximate solutions u_N are measured by the root mean squares (RMS) norm:

$$\text{RMS} = \left(\sum_{z_i \in Z} \frac{(u_N(z_i) - u^*(z_i))^2}{|Z|} \right)^{\frac{1}{2}}, \tag{13}$$

where $Z \in \Omega \cup \partial\Omega$ is a set of regularly placed 101×101 evaluation points.

In Figure 2, we demonstrate the RMS errors for various h from 2×13^{-1} down to 2×115^{-1} with $c = 1.0$ and $c = 0.5$. Also, for each test, the number of selected RBF centers are presented. Thanks to the matrix-free feature, the evaluations of the full matrices (of size up to $116^2 \times 116^2$) are not needed. Moreover, such matrix-free feature makes the collocation method numerically feasible to problems in higher-dimensions.

Also note that both tested c values are relatively large for the original Kansa's method. It can be expected that, for all test cases, the condition numbers of the full matrices are too large

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to be handled by direct solvers in double precision. Furthermore, sizes of some tested matrix systems are too large to be stored.

For both $c = 1$ and $c = 0.5$, the new-Greedy clearly outperforms the old-Greedy over all the tests. Moreover, the new-Greedy shows clear convergence patterns (before stagnation occurs) as h decreases. This is considered to be an improvement over the old-Greedy: when $c = 1$, it is clear in the error profile of the old-Greedy that providing more points as candidates does not always result in better accuracy; particularly in the range of large h's in which the conditioning is comparably well. What we can see is that the RMS errors of old-Greedy first oscillate then stagnate when h decreases.

Another improvement of the new-Greedy is the ability to select more RBF centers when more candidates are provided. Recall that the selection algorithm stops when the resultant Kansa's submatrix, corresponding to the selected centers, is ill-conditioned that potentially harmful to the linear solver. From this point of view, the new-Greedy is better since the number of selected RBF centers are consistently larger than that from the old-Greedy. Also, note that the accuracy is closely related to the number of RBF centers used for the final approximation[‡]. Namely, more RBF centers being selected will usually result in better accuracy.

For a second-order method to achieve an accuracy to the order of 10^{-5} in a 2D problem, over 10^5 nodes/elements are needed. Also presented in Figure 3 is the estimated convergence rate based on the number of candidates N (not the number of selected RBF centers). Although we cannot observe any evidence for exponential convergence with the new-Greedy (with respect to the number of candidates), high convergence rates are observed; namely, 8.2 and 9.6, respectively, for $c = 1.0$ and $c = 0.5$. We have no intention to make any conjecture about the convergence rate of the adaptive algorithm here; the convergence of various modified Kansa's methods addressed by our more theoretical works [30, 37]. On the other hand, it is interesting to note that RBF method [10] results in $\mathcal{O}(h^7)$ and with preconditioning [3, 28] results in $\mathcal{O}(h^{1.78})$ convergence numerically; it is even slower if one employed the domain decomposition method [27]. Effectively, the numerical results in this paper only use a very small subset of the provided N RBF centers; even so, the rate of convergence is faster than the cases when all RBF centers are being used. It is important to have a *good* set of RBF centers instead of *many* RBF centers.

In Figure 3, with $h = 2 \times 115^{-1}$, we demonstrate the RMS errors for various c between 0.5 to 2.5. Note that we are not presenting the so-called c-convergence as the actual number of bases used differs from case to case.

As mentioned in the introduction, having a good shape parameter is important to the accuracy of MQ-RBF method. More importantly, bad shape parameters, usually the ones that are too large, cause the linear solver to break down and results in poor or even unacceptable solution's quality. We want to show that, with the adaptive algorithm, a bad shape parameter will not lead to numerical tragedy. Of course, we want to demonstrate that the new algorithm outperform the previous version.

Each test run has over ten thousand RBF centers as candidates; the numbers of selected RBF centers are relatively small. Obviously, the new-Greedy is better than the old-Greedy not only because of the smaller RMS errors. Moreover, the new-Greedy has the ability to select

[‡]One can still see Equation (2) as an expansion of N basis; but zero coefficients are assigned to the unselected RBF centers.

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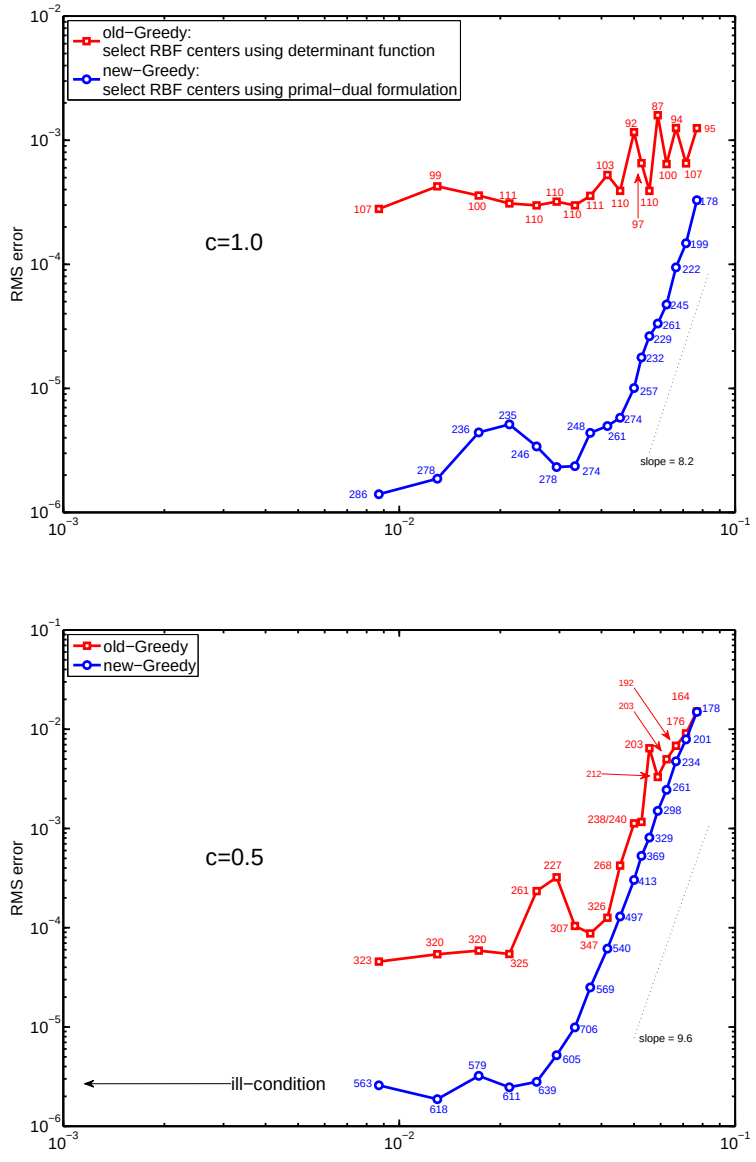

Figure 2. Example 1: RMS errors for different separating distances on RBF candidates; also, provided the number of actually selected RBF centers.

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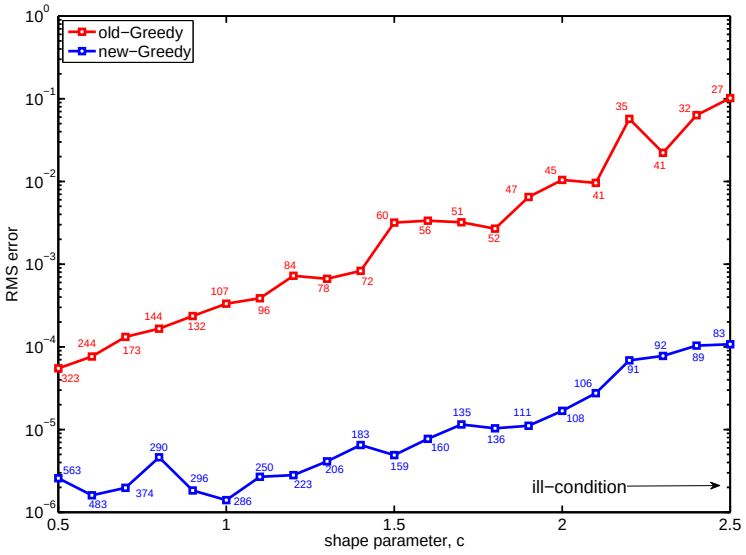

Figure 3. Example 1: RMS errors for different MQ shape parameters.

more RBF centers for large c. In particular, when $c = 0.5$ the new-Greedy selects 1.7× more centers than the old-Greedy; when $c = 2.5$, the new-Greedy selects 3× more. With the higher degrees of freedom, the RMS errors of the new-Greedy is one and three orders of magnitude smaller, respectively, for $c = 1.0$ and $c = 0.5$.

3.2. Example 2

In this example, we solve another 2D Poisson equation with, in (12), $f(x) = -1$ and

$$g(x) = g(x_1, x_2) = \begin{cases} (1 - x_1^2)^2, & \text{if } x_2 = -1, \\ 0, & \text{otherwise.} \end{cases}$$

Since the functions f and g are not generated from an *a priori* known solution, we do not have the *exact solution* for computing error. Note that weak singularities are expected at the corners; e.g., the exact solution does not lie in the native space of the RBF kernel. The numerical set up here is almost the same as in Example 1 except that we increase the weighting on the boundary conditions imposed to the bottom edge of the square. This is to make sure that the incompatible boundary condition is well approximated in the least-squares process.

On a mesh with 40257 nodes and 79872 triangles, the *Matlab Partial Differential Equation Toolbox* is able to solve Example 1 to an accuracy of 6×10^{-5} RMS error (on nodes). We employ the same mesh in this example to generate the approximated solution for evaluating error, see Figure 4. Formula (13) will be used with Z being the 40257 nodes in the mesh.

Due to the presence of singularities, all previous convergence theories on strong from RBF-PDE (reviewed in Section 1) do not hold. For fixed $c = 1$ with various separating distances, the (estimated) RMS errors range between 7.1×10^{-3} to 3.9×10^{-4}, and, the numbers of selected

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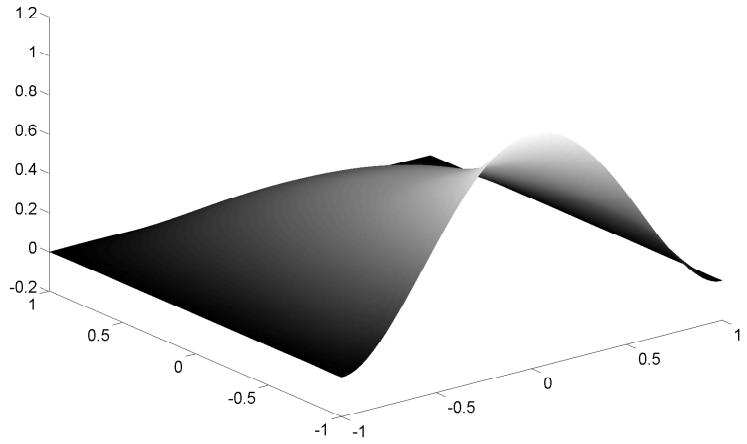

Figure 4. Example 2: Solution obtained by FEM is used to measure error of the proposed method.

basis are between 163 to 401. Both old- and new-Greedy do not provide highly accurate results. To better understand the situation, we will examine the error functions. For separating distance $h = 24^{-1}$, the error functions of both approaches are shown in Figure 5. The maximum errors are 1.25×10^{-2} and 1.30×10^{-2}, respectively, for the old- and new-Greedy. In fact, old-Greedy has smaller maximum error here. Roughly speaking, old-Greedy provides a rather uniform error function that is nice for an one step approach. If high accuracy is not desired, old-Greedy can efficiently provide the user a numerical approximation. On the other hand, new-Greedy results in large error near the corner singularities.

In Figure 6, the error profiles for different shape parameters c are shown. Compared with that in Example 1, see Figure 3, the error reduction is not as obvious. In fact, the error profiles are all similar to the one shown in Figure 6 for different value of c. However, small c does results in more selected basis. Hence, for problems with incompatible boundary conditions, new-Greedy with a large c can be seen as an efficient approach to obtain a smooth approximation. If one then take the residual (with some large c) and apply the greedy algorithm with compactly supported RBFs [15], the *localized errors* can be quickly reduced and results in better numerical solution.

3.3. Example 3

In the last example, the performance of new-Greedy in solving 3D problems are demonstrated. The set of collocation points is regularly spaced in $\Omega = [-1, 1]^3$ with spacing $(2k + 2)^{-1}$ for $k = 1, \ldots, 6$. The set of trial candidates is identical to the collocations points in order to reduce memory requirement. The RMS errors are computed based on a set of regularly placed points

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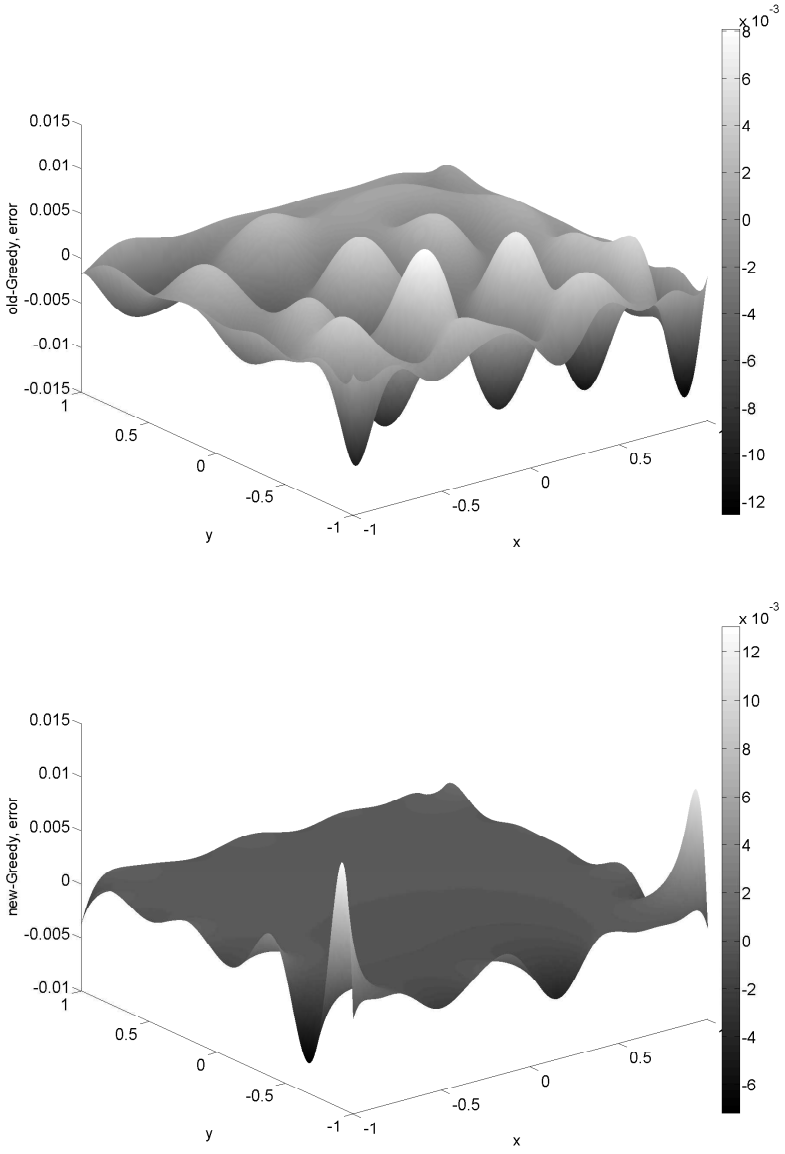

Figure 5. Example 2: Error functions of old-Greedy (#RBF=80) and new-Greedy (#RBF=314) when solving a Poisson equation with singularites.

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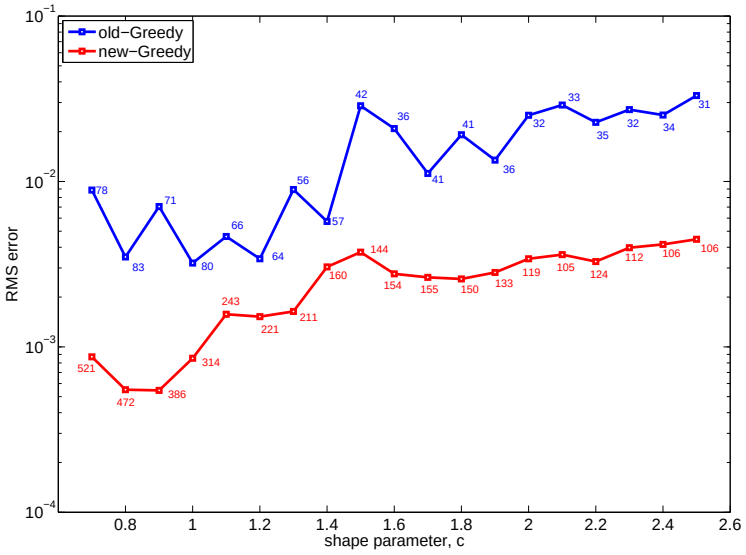

Figure 6. Example 2: RMS differences to the FEM solution for different MQ shape parameters.

with spacing 0.05. Three different exact solutions for (12) are considered:

$$\begin{aligned} u_1(x) &= \frac{1}{\|(x,y,z)^T - (2,2,2)^T\|_2}, \\ u_2(x) &= \exp(x+y+z), \\ u_3(x) &= \cos(x)\cos(y)\cos(z). \end{aligned}$$

In Table I, the RMS errors for different c are shown. As observed in the 2D examples, new-Greedy works extremely well on smooth solutions. We also observed that using $c = 4$ and $c = 1$ results in similar accuracy but the numbers of selected trial centers (e.g. run time) differ by a great amount.

If incompatible boundary conditions and inhomogeneous term are imposed, we will expect a similar loss of accuracy as in Example 2. The result presented here gives a strong motivation to couple the proposed method with the local scheme in [15]. In general, we can expect good approximation from new-Greedy with very localized error; probably near the singularities. In 3D, this smooth approximation will greatly speed up the convergence of the local scheme as it takes away most of the "energy" from the residual. We will leave this to our future work.

4. Conclusion

We presented an improved adaptive algorithm for the unsymmetric radial basis functions (RBFs) collocation method. The proposed algorithm selects a small subset of RBF centers that ensure stable solution. The proposed algorithm is tested against a previously proposed

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$c = 1$			
h	u_1	u_2	u_3
0.2500	7.9E-5 (122)	5.1E-3 (125)	4.1E-4 (125)
0.1667	1.1E-5 (315)	5.1E-4 (320)	5.5E-5 (300)
0.1250	2.2E-6 (531)	8.2E-5 (589)	1.0E-5 (474)
0.1000	4.4E-7 (711)	9.1E-5 (577)	1.9E-6 (607)
0.0833	2.2E-7 (800)	3.4E-5 (724)	2.8E-6 (568)
0.0714	3.9E-7 (721)	2.0E-5 (833)	1.2E-6 (800)

$c = 2$			
h	u_1	u_2	u_3
0.2500	5.0E-5 (125)	2.0E-3 (125)	1.2E-4 (125)
0.1667	2.1E-6 (194)	8.8E-5 (229)	4.4E-6 (208)
0.1250	5.8E-7 (266)	1.9E-5 (285)	1.8E-6 (246)
0.1000	1.8E-6 (245)	7.3E-5 (267)	6.6E-7 (276)
0.0833	1.2E-6 (263)	5.2E-5 (279)	1.1E-6 (265)
0.0714	1.9E-6 (273)	6.6E-5 (292)	1.2E-6 (267)

$c = 4$			
h	u_1	u_2	u_3
0.2500	2.0e-5 (089)	8.5e-4 (091)	1.4e-5 (091)
0.1667	8.2E-6 (103)	7.9E-4 (085)	2.8E-6 (113)
0.1250	6.1E-6 (122)	2.9E-4 (112)	9.7E-6 (102)
0.1000	1.5E-5 (107)	2.4E-4 (110)	6.5E-6 (123)
0.0833	1.1E-5 (114)	3.4E-4 (118)	9.6E-6 (120)
0.0714	1.2E-5 (117)	4.2E-4 (115)	6.1E-5 (076)

Table I. Example 3: RMS errors of new-Greedy with $c = 1, 2, 4$ for some 3D examples. The notation "*aE-e (n)*" stands for an RMS error of $a \times 10^{-e}$ with n selected basis in the least-squares approximation.

algorithm and demonstrates improvements in many different aspects. (1) it demonstrates convergent error profiles as the separating distance decreases; and, (2) the stable error profiles as the RBF shape parameter increases. Moreover, the proposed algorithm is easier to implement and computationally more efficient than the old algorithm. Both 2D and 3D examples are provided. Interested readers are referred to [24] for numerical results when the proposed algorithm is applied to both 2D and 3D modified Helmholtz problems. In [22], the proposed method is coupled with a *periodic* MQ-RBF and the level-set method for simulating 2D combustions.

The proposed algorithm is efficient for solving partial differential equations with smooth solution. However, we emphasize that infinitely-flat RBFs are out of the reach of the proposed algorithm. It is an application dependant problem to get a balance between human labor for implementation, desired accuracy, applicability to irregular domain, and etc. The presented work provides the readers an alternative way to implement the unsymmetric collocation

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method and other meshless methods. It is ideal to handle 3D problems with smooth solution on irregular domains.

Away from singularities, the proposed algorithm is able to well approximate the solution. The numerical solution can be better approximated using compactly supported basis. For time dependent problem, it makes sense to make use of the previously selected RBF centers (enlarge the set if necessary) as candidates for the next time step. Such procedure can reduce the number of candidates and hence reduce complexity of the algorithm. We leave this to our future research.

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