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Improved multiquadric approximation for partial differential equations

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Based on the idea of the DRM, a numerical method has been devised to interpolate the forcing term of partial differential equations by using multiquadric approximations, a special class of radial basis functions, and then use them to approximate particular solutions. To obtain a good shape parameter of the multiquadrics, we use the technique of cross validation. After we find a particular solution, we then use the method of fundamental solutions to solve the homogeneous PDEs. To demonstrate the effectiveness of our method, four numerical results, including a 3D case, are given. Copyright © 1996 Elsevier Science Ltd

Key words: Dual reciprocity method, boundary element method, multiquadrics, cross validation, fundamental solutions, particular solutions.

1 INTRODUCTION

Since the development of the dual reciprocity method (DRM) by Brebbia and Nardini,[1] the boundary element method (BEM) have become an increasingly useful method for the numerical solution of partial differential equations. The idea behind the DRM is the transformation of domain integrals to equivalent boundary integrals by interpolating the forcing term by a series of global basis functions. During the past decade, the DRM has been successfully applied to a wide variety of problems in science and engineering.[2] Traditionally, the *ad hoc* trial function $1+r$ has been used in the DRM without obvious reasons for its choice. Recently, some researchers have considered the choice of trial functions in order to improve the accuracy of the method. Golberg and Chen[3] suggest that the theory of radial basis functions (RBF) provides a mathematical basis for the choice of trial functions in the DRM and numerical work by Golberg,[4] Chen[5] and Karur and Ramachandran[6] have confirmed that the choice of thin plate splines improves the accuracy and efficiency of this technique.

In recent years, the theory of RBFs has undergone intensive research and enjoyed considerable success as a technique for interpolating multivariate data and functions. In 1982, Franke[7] published a review paper evaluating virtually all of the interpolation methods for scattered data sets available at that time. Among the methods tested, Hardy's multiquadrics (MQ) were ranked the best in accuracy, followed by Duchon's thin plate splines. During the past decade, MQ and thin plate spline interpolation have continued to receive considerable attention from the science and engineering communities.

Even though thin plate splines have been considered as optimal for interpolating multivariate functions, they converge only linearly.[8] Because of this, we consider the implementation of MQ approximation in this paper due to its exponential convergence rate.[9]

However, despite MQ's excellent performance, it contains a free parameter, often referred to as the shape parameter, whose choice can greatly affect the accuracy of the approximation. How to choose the optimal shape parameter is a problem that has received the attention of many researchers. So far, this is an open question and no mathematical theory has been developed for determining the optimal value. However, there are various empirical results which have shown success in interpolating multivariate functions. Recently, Milroy *et al.*[10] have developed an exclusion algorithm to automatically choose the optimal shape parameter, which is called cross validation in the statistical literature. Based on their approach, it is the purpose of this paper to implement the MQ as a RBF to interpolate the forcing term of Poisson-type partial differential equations. By doing so, we reduce the problem to a homogeneous differential equation which can be solved by a standard BEM. In recent years, the method of fundamental solutions (MFS) has proved to be an effective boundary method,[5,11,12] and numerical results have shown that the MFS outperforms the BEM in accuracy and efficiency. In this paper, we will use the MFS to solve the homogeneous PDEs.

In section 2, we introduce the general concept of RBFs to approximate the forcing term of differential equations and then use them to approximate the particular solution. In section 3, we choose MQs as a special class of RBFs. An algorithm based on statistical cross validation has been used to search for a good shape parameter. In section 4, we briefly review the MFS. Four numerical examples, including a 3D problem, are given in section 5 to illustrate the effectiveness of our proposed method. We also compare our results with previous methods.

2 RBF APPROXIMATION FOR PARTICULAR SOLUTIONS

The method developed in this section, the method of particular solutions (MPS), evolved from the idea used in the DRM to interpolate the forcing term by a series of radial basis functions. Even though these two approaches are theoretically equivalent under various conditions, we believe that the MPS has some computational advantages over its counterpart, the DRM. We will discuss the computational details after we review the MPS.

For simplicity, let us consider the Dirichlet problem for the Poisson equation

$$\Delta u(P) = b(P), \qquad P \in D \tag{1}$$

$$u(P) = g(P), \qquad P \in \partial D \tag{2}$$

where D is a bounded domain in $\mathbf{R}^n$, ∂D is the boundary of D, and b and g are given functions. To solve (1) and (2) numerically, it is convenient to reduce it to an equivalent homogeneous equation so that BEM techniques can be applied. Let u_{p} be a particular solution of (1), i.e.

$$\Delta u_{\mathrm{p}}(P) = b(P), \qquad P \in D \tag{3}$$

Then $u = v + u_{\mathrm{p}}$ where v satisfies the following homogeneous equation:

$$\Delta v(P) = 0, \qquad P \in D \tag{4}$$

$$v(P) = g(P) - u_{\mathrm{p}}(P), \qquad P \in \partial D \tag{5}$$

Once the particular solution u_{p} has been found, it is routine to solve the boundary value problem (4) and (5) by a standard BEM. In contrast to the DRM approach, this divides the problem into two simpler and independent systems of equations which is more favorable in terms of roundoff error and efficiency. The major difficulty of the MPS is to numerically determine the particular solution u_{p}.

If b in (1) is simple, then u_{p} may be determined analytically. To compute particular solutions for more general bs, we consider the approach used in the DRM which assumes that b can be approximated sufficiently accurately by a series of globally defined basis functions $\{\phi_i\}_{i=1}^N$, i.e.

$$b \simeq \sum_{i=1}^{N} a_i \phi_i \tag{6}$$

where $\{\phi_i\}$ is a set of RBFs and $\{a_i\}$ are the expansion coefficients. Observe that one of the differences of the MPS over the DRM is that we are allowed to choose the collocation points freely without restricting them to be completely inside or on the boundary of the domain. Since particular solutions are not required to satisfy the boundary conditions, we can extend the domain to a rectangular box containing the domain and the interpolating nodes can be easily placed on a uniform grid in this box. The modeling time is then dramatically reduced, especially for irregular domains (see Fig. 1) and/or 3D cases.

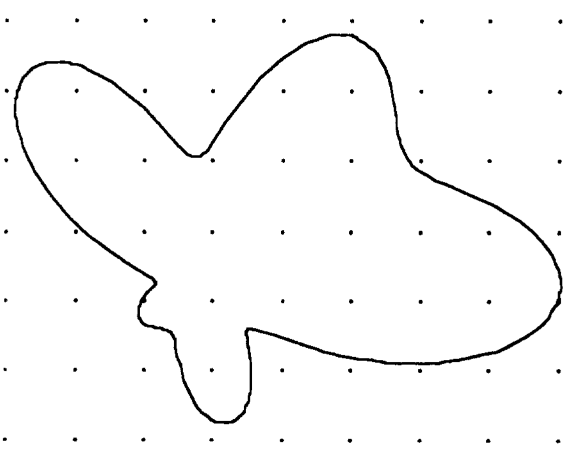

Fig. 1. Unform grid points for surface interpolation.

Next we use the main idea of the DRM to find an approximate particular solution. Replacing b by the series of RBFs in (6), we obtain an approximation $\hat{u}$ for u_p as the solution to

$$\Delta\hat{u}(P) = \sum_{i=1}^{N} a_i\phi_i(P) \tag{7}$$

Since (7) is a linear equation, we have, by superposition,

$$\hat{u}(P) = \sum_{i=1}^{N} a_i\Psi_i(P) \tag{8}$$

where Ψ_i satisfies

$$\Delta\Psi_i(P) = \phi_i(P) \quad \text{for } i = 1, 2, \ldots, N \tag{9}$$

A careful selection of the RBFs $\{\phi_i\}$ is crucial in order that $\{\Psi_i\}$ in (9) can be obtained analytically and b in (6) can be accurately approximated.

To determine $\hat{u}$ in (8) we need to find $\{a_i\}_{i=1}^{N}$. One way to do this is by collocation. Hence let $\hat{D}$ be the minimal rectangle containing D and $\{P_i\}_{i=1}^{N}$ a set of uniformly distributed points in $\hat{D}$. Then we have

$$\sum_{i=1}^{N} a_i\phi_i(P_j) = b(P_j) \quad \text{for } j = 1, 2, \ldots, N \tag{10}$$

The system of equations in (10) is symmetric and $\{a_i\}$ can be obtained by Gaussian elimination with partial pivoting.

3 MQ INTERPOLATION

3.1 Background of MQ

In 1971 Hardy[13] proposed the MQs $\phi(r) = (r^2 + c^2)^{1/2}$ to approximate geographical surfaces, gravitational and magnetic anomalies. But MQs were largely unknown to mathematicians until the publication of Franke's[7] review paper. Since then, due to its excellent performance in interpolating surfaces, the use of MQ has spread to many disciplines and MQ approximation has been under intensive study by many researchers. MQ interpolation is a true grid free scheme for approximating surfaces in an arbitrary number of dimensions. Because MQs are continuously differentiable and integrable, they are extremely useful for application to differential equations. As we indicated in the introduction, another reason that has made MQ approximation so attractive to scientists is its exponential convergence rate.

Even though the mathematical analysis of MQ is very difficult,[14] the basic technique of MQ interpolation is easy to implement. Let us consider the case in $\mathbf{R}^2$. Any function b in (6) may be written as,

$$b(P) \simeq \sum_{i=1}^{N} a_i\phi_i(P) = \sum_{i=1}^{N} a_i(r_i^2 + c^2)^{\frac{1}{2}} \tag{11}$$

where $r_i = \| P - Q_i \|$ and the free parameter $c^2 \geq 0$ is referred as the shape parameter because it shifts the basis function values by c from its value at the data point (x_i, y_i). When c is small, the resulting interpolating surface is pulled tightly to the data points, forming a cone-like basis function. As c increases, the peak of the cone gradually flattens. Moderate values of c give rise to bowl-like basis functions; large cs give rise to flat sheet-like basis functions. By adjusting the shape parameter c, the accuracy of the approximation can be considerably increased and many authors have investigated the effect of varying the shape parameter on the shifted surface. Tarwater[15] found that by increasing c, the root-mean-square (RMS) error of the goodness of fit dropped to a minimum and then grew rapidly thereafter. In general, when c becomes large, $c^2 \gg r^2$, the MQ coefficient matrix in (11) becomes ill-conditioned and the condition number becomes an important factor in choosing the shape parameter. Hence a computer with high precision is preferable for MQ interpolation so that the effect of round-off will be reduced to a minimum. To further increase the accuracy of MQ interpolation, Kansa[16] proposed a scheme which allows the shape parameter to vary with the basis function. He observed that the more distinct the entries of the MQ coefficient matrix are, the lower the MQ coefficient matrix condition number becomes, and the better is the accuracy. Hardy's MQ method with a constant shape parameter works well for data with less than 200 points and this is sufficient for the problems considered in this paper. For large scale problems, variable shape parameters and domain decomposition need to be considered for better accuracy and computational efficiency.

A significant result in selecting the shape parameter was found by Carlson and Foley.[17] In contrast to other results, they found that the optimal value of c was most strongly influenced by the magnitude of the function values, the number of data points and their location in the domain has little influence on the optimal value c. They also suggested that some subsets of the data could be interpolated using several values of c and then choosing the value that yields the best approximation to the excluded data points. Milroy *et al.*[10] followed their approach and published an algorithm to automatically search for the optimal c. To the best of our knowledge, their approach is equivalent to the method of cross validation in the statistical literature.[18] Among all the different algorithms published in recent years for choosing the optimal shape parameter c, we believe their approach is the most reasonable.

Similar to augmented thin plate splines,[3,5,6] MQ interpolants can be enhanced with polynomial terms in order to achieve polynomial precision. The augmented MQ approximations can be written as

$$b(x,y) = \sum_{i=1}^{N} a_i(r_i^2 + c^2)^{\frac{1}{2}} + a + bx + cy \qquad (12)$$

where

$$\sum_{i=1}^{N} a_i = \sum_{i=1}^{N} a_i x_i = \sum_{i=1}^{N} a_i y_i = 0 \qquad (13)$$

As indicated in Ref. 17, adding the polynomial terms does not appear to improve the accuracy for non-polynomial functions.

Once the shape parameter has been determined, we obtain the approximate particular solution $\hat{u}$ by solving the Poisson's equation in (9) in polar coordinates

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \Psi_i}{\partial r}\right) = \sqrt{r^2 + c^2} \quad \text{for } i = 1, 2, \ldots, N \qquad (14)$$

Integration of (14) yields

$$\Psi_i(r) = \begin{cases} \dfrac{-c^3}{3}\left[\ln(2c^2) - \dfrac{4}{3}\right], & \text{for } r_i = 0 \\ \dfrac{-c^3}{3}\ln\left(c\sqrt{r_i^2 + c^2} + c^2\right) & \\ +\frac{1}{9}(r_i^2 + 4c^2)\sqrt{r_i^2 + c^2}, & \text{for } r_i \neq 0 \end{cases} \qquad (15)$$

Similarly, for the three dimensional case, we have

$$\Psi_i(r) = \begin{cases} \dfrac{c^3}{3}, & \text{for } r_i = 0 \\ \left(\dfrac{5c^2}{24} + \dfrac{r_i^2}{12}\right)\sqrt{r_i^2 + c^2} & \\ +\dfrac{c^4\left[ln\left(r_i + \sqrt{r_i^2 + c^2}\right) - \ln c\right]}{8r_i}, & \text{for } r_i \neq 0 \end{cases} \qquad (16)$$

4 CROSS VALIDATION

Cross validation has been used for many years as a standard technique for model selection and the determination of model performance in statistics[18] and our algorithm for finding the optimal shape parameter c is based on the exclusion (cross validation) algorithm of Milroy *et al.*[10] with modifications to improve the efficiency of the computation. Their approach is quite reasonable and reliable and yet computationally inefficient. We will show how to improve their algorithm by applying a standard statistical scheme.

Note that our problem is more than just having a good fit of the surface function b. In certain cases, a good approximation of b does not necessarily guarantee a good approximation of u. Other factors such as the condition number and gradient of the solution to the associated differential equation need to be considered with care.

Let us consider, in $\mathbf{R}^2$, a set of interpolating points $S = \{(x_i, y)\}_{i=1}^{N}$ in an extended domain $\hat{D}$ containing D. First, we set aside a point (x_i, y_i) from S and use the remaining $N - 1$ points to form the basis functions

$$\{\sqrt{r_j^2 + c^2}\}_{j=1, j\neq i}^{N-1}$$

and estimate the coefficients $\{a_j\}_{j=1, j\neq i}^{N-1}$ in (8). We then use this estimate to approximate the function value at the deleted point and compute the error between the predicted and actual value of b at (x_i, y_i), i.e.

$$e_{i,-i} = b(x_i, y_i) - \hat{b}_{i,-i}(x_i, y_i)$$

where $e_{i,-i}$ and $\hat{b}_{i,-i}$ are the prediction error and the approximate value of b at (x_i, y_i), respectively, when (x_i, y_i) is removed from the fitting set. We then repeat the above procedure N times. Thus for a given shape parameter c, the model will be fitted N times.

In the statistical literature, PRESS (prediction residual error sum of squares) is defined as

$$\text{PRESS} = \sum_{i=1}^{N} (e_{i,-i})^2 \qquad (17)$$

It is reasonable, in the statistical sense, to choose the shape parameter c giving the smallest PRESS value.

Using collocation, one can see that the above algorithm may be tedious and inefficient. For each given shape parameter c, there are N prediction errors $e_{i,-i}$ to be calculated and each time a system of $N - 1$ equations needs to be solved. When N becomes large, this approach is not practical.

To remedy this drawback of the above approach, we propose the use of the method of least squares. Instead of choosing one collocation data set, we choose two distinct uniformly distributed point sets $S = \{(x_i, y_i)\}_{i=1}^{N}$ and $T = \{(\hat{x}_j, \hat{y}_j)\}_{j=1}^{N+m}$ when $m \geq 1$. The first set S serves to define the basis functions in (11). The second set T serves as the fitting points for cross validation. During the cross validation process, one data point at a time from T will be set aside as we have stated earlier. Thus we have the following $(N + m) \times N$ system of equations to solve;

$$\begin{bmatrix} d_{11} & d_{12} & \cdots & d_{1N} \\ d_{21} & d_{22} & \cdots & d_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ d_{(N+m)1} & d_{(N+m)2} & \cdots & d_{(N+m)N} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} b(\hat{x}_1, \hat{y}_1) \\ b(\hat{x}_2, \hat{y}_2) \\ \vdots \\ b(\hat{x}_N, \hat{y}_N) \end{bmatrix}$$

where $d_{ij} = [(\hat{x}_j - x_i)^2 + (\hat{y}_j - y_i)^2 + c^2]^{1/2}$. In matrix notation, we have

$$\mathbf{D} \cdot \mathbf{A} = \mathbf{B} \tag{18}$$

Removing a data point $(\hat{x}_i, \hat{y}_i)$ in the cross validation process is equivalent to removing the ith row from $\mathbf{D}$ and $\mathbf{B}$. By applying the Sherman–Morrison–Woodbury theorem, it is well known that the computation of PRESS in (17) is quite simple and does not require one to repeatedly remove a row from $\mathbf{D}$ and $\mathbf{B}$.[18]

If $\mathbf{D}^{\mathrm{T}}$ denotes the transpose of the matrix $\mathbf{D}$ and $\mathbf{d}_i$ is the ith row of $\mathbf{D}$, then we can calculate the PRESS residual $e_{i,-i}$ from the original matrix $\mathbf{D}$ without removing a row from it, i.e.

$$e_{i,-i} = \frac{b(\hat{x}_i, \hat{y}_i) - \hat{b}(\hat{x}_i, \hat{y}_i)}{1 - \mathbf{d}_i(\mathbf{D}^{\mathrm{T}}\mathbf{D})^{-1}\mathbf{d}_i^{\mathrm{T}}} = \frac{e_i}{1 - h_{ii}} \tag{19}$$

where $\hat{b}(\hat{x}_i, \hat{y}_i) = \mathbf{d}_i(\mathbf{D}^{\mathrm{T}}\mathbf{D})^{-1}\mathbf{D}^{\mathrm{T}}\mathbf{B}$ and h_{ii} is the ith diagonal element of the HAT matrix $\mathbf{H} = \mathbf{D}\,(\mathbf{D}^{\mathrm{T}}\mathbf{D})^{-1}\mathbf{D}^{\mathrm{T}}$. (We remark that $\mathbf{D}^{\dagger} = (\mathbf{D}^{\mathrm{T}}\mathbf{D})^{-1}\mathbf{D}^{\mathrm{T}}$ is the *pseudoinverse* of $\mathbf{D}$ which can be computed by either the QR decomposition or singular value decomposition (SVD), using software such as MATHEMATICA or MATLAB.) By the definition of PRESS in (17), we have

$$\mathrm{PRESS} = \sum_{i=1}^{N+m} \left(\frac{e_i}{1 - h_{ii}} \right)^2 \tag{20}$$

We refer the reader to Ref. 18 for a detailed derivation of (20).

Equation (20) is quite remarkable in terms of computational cost. It enables one to carry out the algorithm efficiently and choose the optimal value (or a consistently good value) for the shape parameter c from a series of tests. The extra effort needed to select the optimal c is worthwhile, as our numerical results show several orders of magnitude improvement over previous ones.

5 THE MFS FOR LAPLACE EQUATION

Once the approximate particular solution $\hat{u}$ has been computed, it is straightforward to solve the Dirichlet problem (4) and (5). In the past, the BEM has been widely accepted as a method for solving (4) and (5). However, in recent years the MFS has been developed as another effective boundary method.[3,5,12] In the MFS, the solution of a homogeneous equation subject to a nonhomogeneous boundary condition is approximated by a linear combination of fundamental solutions of the governing differential equation. In this method we imbed the domain D into a larger fictitious domain D^* with boundary ∂D^*. We then place source points on ∂D^*.

Let $\{Q_i\}_{i=1}^{M}$ be a set of distinct source points lying on ∂D^* and

$$G(P,Q) = \begin{cases} \dfrac{1}{2\pi} \ln \| P - Q \|, & P, Q, \in \mathbf{R}^2 \\ \dfrac{1}{4\pi \| P - Q \|}, & P, Q \in \mathbf{R}^3 \end{cases}$$

where $\| P - Q \|$ is the Euclidean distance between P and Q and $G(P,Q)$ is the fundamental solution of Laplacian. Then

$$v_M = \sum_{i=1}^{M} c_i G(P, Q_i) \tag{21}$$

may be taken as an approximation to v in (4) and (5). For theoretical reasons,[12,19] it is more appropriate (in the two dimensional case) to add a constant c to v_M giving

$$v_M = \sum_{i=1}^{M} c_i G(P, Q_i) + c \tag{22}$$

The coefficients $\{c_i\}_{i=1}^{M} \cup \{c\}$ are then chosen to satisfy the boundary conditions as well as possible. The simplest way of doing this is by collocation. For this we choose a set of points $\{P_j\}_{j=1}^{M+1}$ on ∂D and then set v_M equal to the boundary conditions in (5) at those points. This gives the system of equations in $M+1$ unknowns:

$$\sum_{i=1}^{M} c_i G(P_j, Q_i) + c = g(P_j) - \hat{u}(P_j),$$
$$\text{for } j = 1, 2, \ldots, M+1$$

It was shown by Bogomolny[19] that if ∂D is analytic and $\{Q_k\}$ are dense in ∂D^*, then $\{G(P, Q_k)\}_{k=1}^{\infty} \cup \{c\}$ are dense in $H(D)$, the set of harmonic functions in D. This means that every solution v to $\Delta v = 0$ can be approximated arbitrarily closely by a function v_M of the type in (22) for M chosen sufficiently large. Bogomolny also showed that ∂D^* could be taken as a circle with radius R and $\{Q_k\}_{k=1}^{M}$ equally spaced around the circle. As indicated by Bogomolny,[19] the larger the radius of the source circle, the better the approximation to be expected. Although at present there does not appear to be a general theory for choosing $\{P_j\}_{j=1}^{M+1}$, Cheng's[20] results showed that it is adequate to choose these points uniformly distributed on ∂D.

This method is remarkably simple and, as our numerical results show, can be highly accurate. We also note that the MFS has none of the integration problems associated with standard boundary integral methods. In particular, we expect uniform convergence to hold up to the boundary, in contrast to the deterioration of convergence expected in the traditional boundary methods.

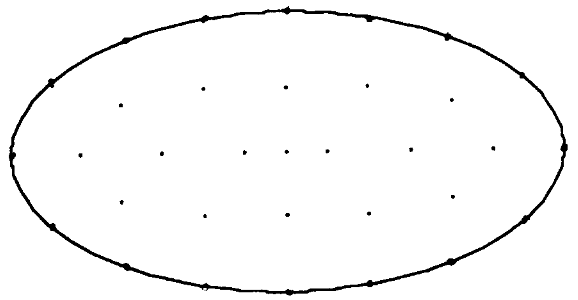

Fig. 2. 16 boundary and 17 interior points in domain D.

6 NUMERICAL RESULTS

Coupling the MFS, MPS and MQ interpolation, we give four examples to demonstrate the accuracy and wide applicability of our proposed technique. All computations in this paper were performed in double precision on a personal computer (GATEWAY 2000, 4DX-33V) with Microsoft Fortran compiler version 5.1. For all examples, we chose $m = 1$ in (20).

Example 1

To compare our proposed method with the DRM using $1 + r$ as the basis function,[2] we consider the following problem

$$\Delta_u(P) = -x^2, \quad P \in D$$
$$u(P) = 0, \quad P \in \partial D$$

where $D = \{(x, y) : x^2 + 4y^2 \leq 4\}$. The analytical solution is given by $u(x, y) = (-50x^2 - 8y^2 + 33{\cdot}6) \times (x^2/4 + y^2 - 1)/246$.

To compute the particular solution we choose the same interpolating points, 16 on the boundary and 17 in the interior of D (Fig. 2), given in Ref. 2. For the MFS, 15 source points are evenly placed on the source circle of radius 8 and we use the 16 interpolating points on the boundary as collocation points. For cross validation, we choose those 33 interpolating points to form the MQ basis functions. The second set of fitting points contains 34 quasi-random points.

Based on the numerical results in Tables 1 and 2, the optimal shape parameter is $c = 4$, yet the best approximation of u seems to occur between $c = 4$ and $c = 10$. Nevertheless, we have a very comfortable range of shape parameters since the difference of these PRESS statistics is insignificant.

Compared with the results in Table 3,[12] one should note that we obtain a thousand-fold decrease in the error over previous methods for the same amount of computational effort.

Example 2

Let us consider the problem

$$\Delta u(P) = 2e^{x-y}, \quad P \in D$$
$$u(P) = e^{x-y} + e^x \cos y, \quad P \in \partial D$$

where $P = (x, y)$ and D is defined as the interior of the Oval of Cassini. Its parametric representation is as follows:

$$x = r(\theta)\cos\theta, \quad y = r(\theta)\sin\theta,$$

$$r(\theta) = \sqrt{\cos 2\theta + \sqrt{1{\cdot}1 - \sin^2 2\theta}}, \quad 0 \leq \theta \leq 2\pi$$

As shown in Fig. 3, we generate 60 quasi-random nodes[11] on a minimal rectangular domain containing D and then used them as collocation points to interpolate the forcing term $2e^{x-y}$ by MQs. The purpose of using quasi-random numbers is to ensure a uniform distribution of the interpolating points. For the MFS, 35 field points are uniformly distributed (in terms of angle) on the boundary, i.e. $\{P_j\}_{j=1}^{35} = \{(r(\theta_j)\cos\theta_j, r(\theta_j)\sin\theta_j)\}_{j=1}^{35}$, where $\theta_j = 2\pi j/35$. Similarly, 34 source points are evenly placed on the source circle with radius R, i.e. $\{Q_i\}_{i=1}^{34} = \{(R\cos\theta_i, R\sin\theta_i)\}_{i=1}^{34}$ where $\theta_i = 2\pi i/34$ and $R = 12$. Two sets of quasi-random

Table 1. PRESS values

c	1	2	4	5	7	10	15	30
PRESS	0·092	0·011	0·002	0·037	0·019	0·0035	0·234	34·70

Table 2. Absolute error in approximation to $u(x, y)$

x	y	$u(x,y)$	$c = 1$	$c = 2$	$c = 4$	$c = 5$	$c = 7$	$c = 10$
1·5	0·0	0·350	4·53E − 4	2·75E − 4	3·98E − 5	1·59E − 5	8·06E − 6	1·55E − 5
1·2	−0.35	0·414	3·08E − 5	6·54E − 5	8·69E − 6	3·07E − 6	1·63E − 6	5·87E − 6
0·6	−0·45	0·566	3·41E − 4	4·14E − 5	4·46E − 6	2·59E − 6	8·46E − 7	3·83E − 6
0·0	0·45	0·638	5·76E − 4	1·03E − 4	1·07E − 6	5·10E − 6	1·87E − 6	1·16E − 6
0·9	0·0	0·638	1·02E − 4	3·02E − 5	4·85E − 6	1·42E − 6	8·67E − 7	7·29E − 7
0·3	0·0	0·782	3·05E − 4	4·64E − 5	5·35E − 6	2·91E − 6	1·14E − 6	5·49E − 6
0·0	0·0	0·800	3·61E − 4	6·68E − 5	7·92E − 6	3·98E − 6	1·15E − 6	2·82E − 7

Table 3. Solutions of $\Delta u = -x^2$ on D

x	y	Analytical solution	MFS/TPS solution	DRM solution	H-bicubic solution
1·5	0·00	0·260	0·261	0·269	0·259
1·2	·35	0·220	0·220	0·220	0·224
0·6	·45	0·144	0·144	0·135	0·140
0·0	·45	0·103	0·104	0·092	0·097
0·9	0·00	0·240	0·240	0·236	0·235
0·3	0·00	0·151	0·151	0·142	0·149
0·0	0·00	0·137	0·135	0·127	0·132

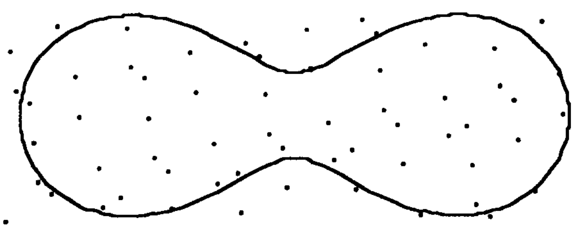

Fig. 3. Showing 60 quasi-random points scattered in and around an Oval of Cassini.

data were generated to find a good shape parameter. The first set consists of 33 points used to define the multiquadric basis functions. The second set consists of 34 points used for fitting and cross validation. The PRESS statistics, are shown in Table 4, indicate that $c = 1{\cdot}5$ is optimal. To demonstrate the accuracy of our method, we evaluated the approximate value of u on eight non-collocation points as shown in Ref. 21. The results in Table 6 (later) showed that the accuracy of this method is as good as the classical methods.

We remark that the good fit for the forcing term as shown in Table 5 does not necessarily result in a better solution u as we have indicated in section 2. For instance, we got a better approximate forcing term at $c = 5$ than $c = 1$ and 1·5 and yet the approximate solution u is much worse at $c = 5$ as shown in Tables 5 and 6. In this example, the smallest PRESS statistic in Table 4 occurred at $c = 1{\cdot}5$ and agrees with the best approximation of u in Table 6.

Table 4. PRESS values

c	0·8	1·0	1·5	2·0	3·0	4·0	5·0
PRESS	2·11	1·34	0·82	1·11	2·47	3·63	3·85

Example 3

To further illustrate the effectiveness of the proposed method, we consider a benchmark problem in Ref. 22. This problem is governed by Poisson's equation

$$\Delta u(P) = \frac{-10^6}{52}, \quad P \in D$$

$$u(P) = 0, \quad P \in \partial D$$

where $D = \{(x, y) : -0{\cdot}3 \le x \le 0{\cdot}3, -0{\cdot}2 \le y \le 0{\cdot}2\}$. The value of u at the center (0, 0) is 310·10.

Since the forcing term is a constant, we choose $\phi_i = \sqrt{r_i^2 + c^2} + a$, where a is a constant, as the basis function in (12). In all, 32 uniformly distributed grid points were placed on the domain D as collocation points for MQ interpolation. To compute the PRESS statistics, one quasi-random set with 33 points and a uniform grid with 32 points were generated. A total of 20 collocation points, (±0·3, 0), (±0·3, ±0·1), (±0·3, ±0·2), (0, ±0·2), (±0·1, ±0·2), (±0·2, ±0·2), were evenly placed on the boundary ∂D and 19 source points were evenly distributed on a circle with radius 1·2. The results in Table 7 shows that the PRESS value, the approximate forcing term $\hat{b}(x, y)$ and the solution u_M do not depend on the shape parameter. The approximation of the forcing term is exact as expected. Most importantly, the approximation of $u(0, 0)$ is highly accurate and consistent with the PRESS value.

Since the constant forcing term can be exactly approximated, no interior points are required for this case. Results in Table 8 show that it requires only 20 boundary points for the interpolation and the result is almost identical to Table 7.

Example 4

To show that our method can be easily applied to three dimensional problems, we consider the following

Table 5. Absolute error in approximation to $b(x, y) = 2e^{x-y}$

x	y	$b(x,y)$	$c = 1$	$c = 1.5$	$c = 2$	$c = 3$	$c = 4$	$c = 5$
0·0	0·0	2·000	4·44E − 5	4·43E − 5	7·33E − 6	2·49E − 6	5·02E − 6	1·00E − 5
0·626	0·0	3·741	1·62E − 4	3·69E − 6	5·29E − 6	1·25E − 7	1·70E − 7	2·11E − 5
1·342	0·0	7·653	3·12E − 3	3·13E − 4	2·80E − 5	2·71E − 5	1·08E − 6	3·92E − 5
0·174	0·174	2·000	2·16E − 4	5·62E − 5	6·57E − 5	3·58E − 6	3·78E − 6	1·20E − 5
0·373	0·373	2·000	2·62E − 4	2·42E − 5	3·67E − 5	7·20E − 6	1·57E − 6	8·49E − 6
0·0	0·207	1·626	3·60E − 4	5·80E − 5	8·28E − 6	1·87E − 6	2·14E − 6	6·84E − 6
−0·373	0·373	0·949	2·28E − 4	2·32E − 5	1·24E − 5	2·88E − 6	7·52E − 6	5·90E − 6
−1·342	0·0	0·523	5·95E − 6	1·80E − 5	1·90E − 7	2·18E − 6	3·77E − 6	7·09E − 6

Table 6. Absolute error in approximation to $u(x,y)$

x	y	$u(x,y)$	$c=1{\cdot}0$	$c=1{\cdot}5$	$c=2{\cdot}0$	$c=3{\cdot}0$	$c=4{\cdot}0$	$c=5{\cdot}0$
0·0	0·0	2·000	7·86E − 7	8·27E − 8	8·94E − 7	5·92E − 6	4·48E − 5	1·00E − 3
0·626	0·0	3·741	5·72E − 6	7·23E − 7	5·25E − 8	3·11E − 6	2·85E − 5	4·48E − 2
1·342	0·0	7·653	3·47E − 5	4·27E − 6	2·50E − 7	6·23E − 6	4·70E − 4	7·67E − 3
0·174	0·174	2·172	8·82E − 6	1·06E − 6	1·29E − 6	5·47E − 6	3·59E − 5	1·25E − 2
0·373	0·373	2·352	1·77E − 7	1·04E − 6	2·13E − 6	8·88E − 7	8·04E − 5	1·55E − 2
0·0	0·207	1·792	3·31E − 6	1·47E − 8	3·16E − 7	1·66E − 6	3·34E − 6	2·55E − 2
−0·373	0·373	1·116	1·16E − 6	8·76E − 7	4·80E − 7	1·60E − 6	6·13E − 6	7·61E − 2
−1·342	0·0	0·523	1·26E − 5	2·12E − 5	2·25E − 6	6·29E − 5	2·81E − 3	7·18E − 1

Table 7. PRESS value, approximated forcing term and solution

c	PRESS	$\hat{b}(0,0)$	$b(0,0)$	$u_M(0,0)$	$u(0,0)$
1	$6{\cdot}5E-17$	1923·077	1923·077	310·160	310·1
3	$1{\cdot}6E-20$	1923·077		310·160	
5	$6{\cdot}5E-21$	1923·077		310·160	
7	$4{\cdot}1E-20$	1923·077		310·156	
9	$1{\cdot}5E-20$	1923·077		310·160	
15	$1{\cdot}4E-20$	1923·077		310·156	
20	$2{\cdot}3E-20$	1923·077		310·160	
30	$2{\cdot}9E-20$	1923·077		310·156	
50	$2{\cdot}7E-20$	1923·077		310·160	
70	$2{\cdot}3E-20$	1923·077		310·160	

problem:

$$\Delta u(P) = 4 - x^2, \quad P \in D$$

$$u(P) = \frac{-x^4}{12} + y^2 + z^2, \quad P \in \partial D$$

where $P=(x,y,z)$ and $D=\{(x,y,z): x^2/4 + y^2 + z^2 \leq 1\}$ is an ellipsoid. Since the boundary conditions satisfy the differential equation, the exact solution is $u(x,y,z) = -x^4/12 + y^2 + z^2$.

To interpolate the forcing term, we generate 60 quasi-random collocation points in a minimal rectangular box containing D which were then used to compute the approximate particular solution. For the 3D case, the constant term in (22) is not necessary. Hence, the number of source and field points are equal. For this we chose 50 equally distributed points on the surface of the ellipsoid and source sphere. The radius of the source sphere were chosen to be 10. To compute the PRESS value, two sets of quasi-random points, containing 50 and 51 nodes each, were chosen. The PRESS values in Table 9 indicate that we expect to get a good approximation if we choose the shape parameter c between 2 and 10. We then evaluate the approximate solution at seven random points as shown in Table 10.

Table 8. Approximate solution of $u(0,0)$ without using interior node

c	1	3	5	7	9	15	30	50
u	310·160	310·156	310·156	310·156	310·160	310·160	310·157	310·159

Table 9. PRESS values

c	1	2	3	4	5	6	7	8	9	10	11	12
PRESS	35·8	0·27	0·03	0·03	0·15	0·11	0·07	0·12	0·19	0·13	0·8	1·33

Table 10. Absolute error in approximation to $u(x,y,z)$

x	0·0	1·2	−0·5	−0·7	0·9	0·0	0·4
y	0·0	0·3	0·3	0·5	0·4	−0·5	−0·4
z	0·0	0·1	−0·2	0·2	0·1	0·5	0·21
$u(x,y,z)$	0·00	−0·0728	0·1248	0·2700	0·1153	0·5000	0·2020
$c=1$	3·6E − 4	1·5E − 2	2·4E − 4	9·9E − 3	1·1E − 2	4·5E − 12	1·6E − 3
$c=3$	1·2E − 4	1·4E − 3	3·0E − 4	5·2E − 4	1·1E − 3	9·5E − 13	4·1E − 4
$c=5$	4·5E − 5	9·0E − 5	1·4E − 4	3·7E − 6	2·2E − 4	1·1E − 12	1·2E − 4
$c=7$	1·7E − 5	2·3E − 4	7·6E − 5	4·6E − 6	3·5E − 5	7·4E − 13	7·6E − 5
$c=9$	9·6E − 7	4·0E − 4	4·4E − 5	1·6E − 5	3·2E − 5	1·0E − 12	7·0E − 5
$c=11$	1·0E − 5	5·6E − 4	2·5E − 5	3·2E − 5	7·3E − 5	2·3E − 12	8·6E − 5
$c=12$	1·6E − 5	6·5E − 4	1·8E − 5	4·3E − 5	8·9E − 5	4·5E − 13	9·8E − 5

The results show the consistency between the PRESS value and the approximation to u.

7 CONCLUSIONS

Multiquadrics is a powerful method in multivariate interpolation. In this paper we have demonstrated that MQ approximation is highly accurate if we can find a good shape parameter. Even though the optimal shape parameter is still not available, the approach of cross validation provides us with a reasonable way of finding a good shape parameter. Equipped with the MQ approximation, we were able to approximate the particular solution accurately. Coupled with the MFS, the numerical results have improved significantly. Furthermore, the MFS and MQ method can be easily extended to the problems in arbitrary dimensions and the basic technique of this paper can be applied to various type of elliptic partial differential equations and boundary conditions.

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