Highly accurate methods for solving elliptic and parabolic partial differential equations

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Abstract

This paper is a study of two approaches to obtain very high accuracy in time-dependent parabolic partial differential equations (PDEs) with the use of the C^∞ multiquadric (MQ) radial basis functions (RBFs). For the spatial part of the solution, the MQ-RBF is generalized having the form, $\phi_j(\mathrm{x}) = \{(\mathbf{x}\text{-}\mathbf{x}_j)^2 + c_j^2\}^\beta$ and $\beta > -1/2$ can be either a half integer, or any number, excluding a whole integer. The other shape parameter, c_j^2, is allowed to be different on the boundary and the interior, and is permitted to vary with odd and even values of the index, j. The temporal and spatial variations of the solution, U($\mathbf{x}$,t) are treated by the separation of variables in which the temporal portion is accounted by the expansion coefficients and the spatial portion is accounted by the MQ-RBFs. It was observed that the PDE on the interior is really a system of time dependent ordinary differential equations (ODEs) with either stationary or non-stationary constraints on the boundary. The solution of the time advanced expansion coefficients both on the interior and on the boundary can be accomplished by analytical methods, rather than by low order time advanced schemes.

1 Introduction

The interest in mesh-free methods to solve PDEs has grown considerably in the past 15 years. The two principal reasons are: (1) Mesh generation over complicated two and three dimension domains may require weeks or months to produce a well behaved mesh, and (2) The convergence rate of traditional methods are typically second order in space and time. The mesh-free radial basis functions (RBFs) have been shown to be particularly attractive by Fedoseyev et al. [1], and Cheng et al. [2] because of the exponential convergence of certain C^∞ RBFs that has been

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observed. One of the most used RBFs is the multiquadric RBF. The generalized MQ basis function, $\phi_j(\mathbf{x})$, where $\mathbf{x} \in \Re^d$ is given by

$$\phi_j(\mathbf{x}) = [(\mathbf{x} - \mathbf{x}_j)^2 + \mathrm{c}_j^2]^\beta. \tag{1}$$

Commonly used values for β are -1/2 and 1/2. Madych and Nelson [3] and Madych [4] have proven theoretically that MQ interpolation converges exponentially as $\eta^{(c/h)}$ where $\eta < 1$, and h = $\max|(\mathbf{x_i} - \mathbf{x}_j)|$. For any continuous function, U($\mathbf{x}$), over the domain, Ω, can be expanded as

$$\mathrm{U}(\mathbf{x}) = \sum_{j=1}^{N} \phi_j(\mathbf{x})\alpha_j + \sum_{k=1}^{M} \mathrm{p_k}(\mathbf{x})\gamma_k \tag{2}$$

where $\mathrm{p_k}(\mathbf{x})$ is a polynomial of degree k,and the expansion is subject to the constraint conditions:

$$\sum_{j=1}^{N} \mathrm{p_k}(\mathbf{x})\alpha_j = 0 \tag{3}$$

Hyperbolic, parabolic, or elliptic partial differential equations (PDEs) can be solved by an analogy to the interpolation problem, see [5]. Given the operators $\mathcal{L}$ on the interior, $\Omega\backslash\partial\Omega$, and the boundary condition operator, ß, on the boundary, $\partial\Omega$, where ß may represent a Dirichlet, Neumann, or Robin operator, the PDE problem is formulated as:

$$\mathcal{L}\mathrm{U} = \sum_{j=1}^{N} \mathcal{L}\phi_j(\mathbf{x})\alpha_j + \sum_{k=1}^{M} \mathcal{L}\mathrm{p_k}(\mathbf{x})\gamma_k = \mathrm{f} \;\text{ on } \Omega\backslash\partial\Omega, \tag{4}$$

$$\text{ß}\mathrm{U} = \sum_{j=1}^{N} \text{ß}\phi_j(\mathbf{x})\alpha_j + \sum_{k=1}^{M} \text{ß}\mathrm{p_k}(\mathbf{x})\gamma_k = \mathrm{g} \;\text{ on } \partial\Omega, \tag{5}$$

subject to the constraints

$$\sum_{j=1}^{N} \mathcal{L}\mathrm{p_k}(\mathbf{x})\alpha_j = 0, \text{ and} \tag{6}$$

$$\sum_{j=1}^{N} \text{ß}\mathrm{p_k}(\mathbf{x})\alpha_j = 0. \tag{7}$$

When U(x), given by Eq(2), is inserted into Eqs (4-7), a system of linear or nonlinear equations is obtained, and we can obtain the expansion coefficients, $[\alpha, \gamma]^T$ to recover the expansion of U($\mathbf{x}$) by Eq(2). Because the asymmetric collocation method is based upon interpolation, an acceptable degree of convergence can be achieved either by increasing c_j^2 or decreasing h; however the price is usually the ill-conditioning problem resulting from the use of Gaussian elimination methods to find the expansion coefficients.

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Standard low order finite difference, element and volume methods give rise to banded system of equations whose bandwidth increases with the number of dimensions. Since the convergence is typically second order, the system of equations requires a larger number, N, of discretization sites, and the resulting system of equations is very ill-conditioned. Hence, special methods such as domain decomposition and specialized preconditioners are used. Because 5-8 orders of magnitude of equations need to be solved, only those organizations that have access to super computers can attempt to solve large scale problems. The viable alternative investigate how RBFs may achieve accelerated convergence, so orders of magnitude of courser discretization may be used.

Although many papers have shown MQ to be a powerful tool, there is no widely accepted theory or recipe for choosing the optimal shape parameters for various applications. This problem has been investigated by several authors such as Hardy [6], Foley [7], Carlson and Foley [8], Kansa and Carlson [9], Golberg et al. [10], Rippa [11], and Kansa and Hon [12].

Bengt Fornberg and co-workers [13,14,15,16] have written a series of papers investigating the convergence rates of C^∞ RBFs such as the Gaussian and MQ RBFs in the limit of infinitely flat basis functions. They have shown extraordinary convergence rates of these basis functions for both interpolation and PDE problems, and have found these RBFs have removable singularities in the complex plane with polynomial limit behavior.

Wang and Liu [17] , Xiao and McCarthy [18] and Xiao et al. [19] expanded the definition of the MQ shape parameter to include not only c^2 ,but the MQ exponent, β, as an additional parameter to be optimized.

Recently, Ling and Kansa [20, 21] and Brown et al. [22] showed that an approximate least squares cardinal function (LSCF) preconditioner can be constructed that transforms an ill-conditioned system of equations arising from PDE systems using RBFs into a well conditioned system such that the unknown expansion coefficients could be found by GMRES iterations. The authors solved problems in $\Re^2$ and found empirically that the constant, $c = k/\sqrt{N}$,where N is the total number of points, and k may safely range up to 5. Furthermore, they found, with increasing numbers of subdomains, that the additive Schwarz algorithm not only reduces the operation count, but increases the convergence rate. Most recently, Ling and Hon [23] developed an affine space decomposition scheme for solving linear equations that is extremely stable, because the small eigenvalue components are projected away. This has proven to be stable even for a full system of equations having a rank of over 1000. When combined with domain decomposition, this tool should be extremely useful for simulating very large complex systems of PDEs.

2 The role of shape parameters

This paper builds upon several observations. The first is the observation of Fedoseyev et al. [1] that a PDE exists not only on the domain, Ω, but also slightly beyond its boundary, $\partial\Omega$. A boundary can be interpreted as a constraint condition upon the PDEs at specific locus. So interior points may not only coincide with

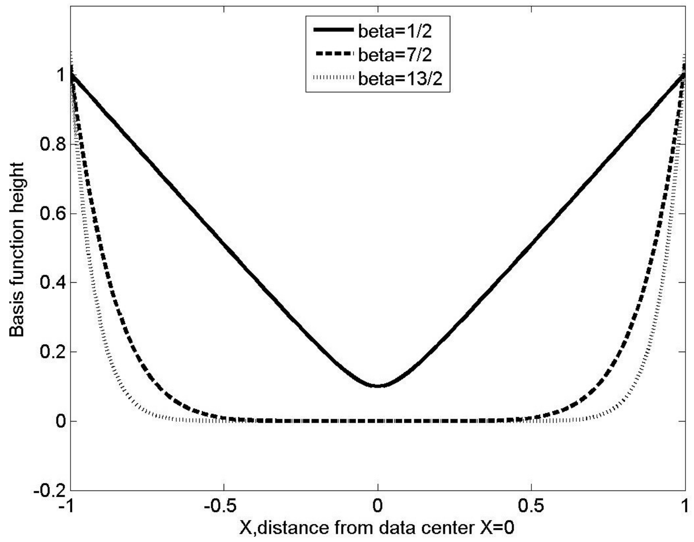

Figure 1: An illustration of three MQ basis functions with β = 0.5 , 3.5 and 6.5 over [-1,1].

boundary points, but extended slightly beyond $\partial\Omega$.

Consider the generalized MQ basis function in a hyperplane in $\Re^d$, given by Eq(1). The term, $\{(\mathbf{x}\text{-}\mathbf{x}_j)^2\text{+c}_{j,}^2\}$, is the squared Euclidian metric distance in the space, $\Re^{d+1}$. Then, c_j, can be interpreted as a distance in the (d+1)th dimension. The optimal solution on the hyperplane in $\Re^d$ will depend upon the distance in the direction normal to the hyperplane. We seek to find the minimum potential energy for this distribution.

Hence, we postulate that the squared distance should be raised to the power, β, that will be found by optimization. Figure 1 shows the plots of two basis functions each with c^2=0.01, but with the exponent β=1/2 and 7/2 centered at x=0. Notice the β=1/2 basis function is a rounded conic shape rising linearly away from the data center, but the β=7/2 and 13/2 RBFs are flattened near x=0, and rises very rapidly near x = $\pm$1. For large distances away from the data center, the asymptotic forms behave as the polynomials $\mathbf{x}$, $\mathbf{x}^7$ and $\mathbf{x}^{13}$, respectively. When solving partial differential equations, it is important to remember that spatial differentiation of the basis function reduces the order of the basis function, irrespective of the dimensionality of the space. Asymptotically, $\phi_j(\mathbf{x})$=$\{\mathbf{x}^2\text{+c}^2\}^\beta \rightarrow \mathbf{x}^{2\beta}$, $\phi_j'(\mathbf{x}) \rightarrow \mathbf{x}^{2\beta-1}$,$\phi_j''(\mathbf{x}) \rightarrow \mathbf{x}^{2\beta-2}$, etc., where the number of primes indicate the order of differentiation. If we wish to approximate ∇^2U by at least a quadratic function, and if $\beta \geq$ 7/2, then $\nabla^2\phi_j(\mathbf{x})$ will be at least quadratic.

Because there can be an infinite number of solutions to Eq(4), the boundary conditions, Eq(5), force the solution to be unique. Since the boundary conditions have such an important influence upon the solution over the entire domain, we allow the c_j^2 distances to be different and possibly much larger than those associated with the interior problem, especially when Dirichlet conditions are applied. A large value of c_j^2 also makes the MQ basis function locally flatter. It was observed in [5] that a variable c_j^2 distribution based upon a power law distribution performs optimally for strictly monotonic increasing or decreasing functions. In [12], it was hypothesized that the c_j^2 distribution may be related to the local radius of curvature, it was not seriously considered because of the computational effort to calculate the local radius of curvature.

The optimization of the MQ shape parameters was studied on two Poisson problems: The first is

$$\nabla^2 \mathrm{U} = 8e^{2x+2y}, \tag{8}$$

on a domain, Ω, represented by a unit square with Dirichlet boundary conditions on all four sides. The exact solution is $\mathrm{U}=e^{2x+2y}$. The second is

$$\nabla^2 \mathrm{U} = -8\pi^2 \cos(2\pi\{x+y\}), \tag{9}$$

on a domain, Ω, represented by a unit square, with Dirichlet boundary conditions on all four sides. Its exact solution is $\mathrm{U}= \cos(2\pi\{x+y\})$.

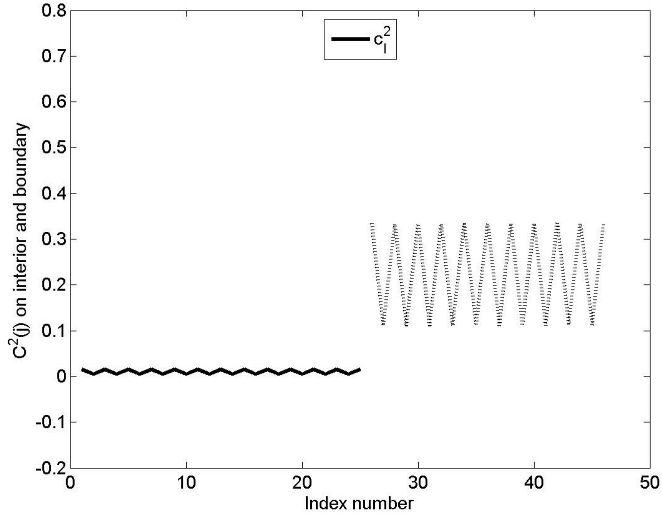

Figure 2: A typical distribution of a optimized distribution of oscillating $c^2_{\Omega\backslash\partial\Omega} << c^2_{\partial\Omega}$ (not to scale).

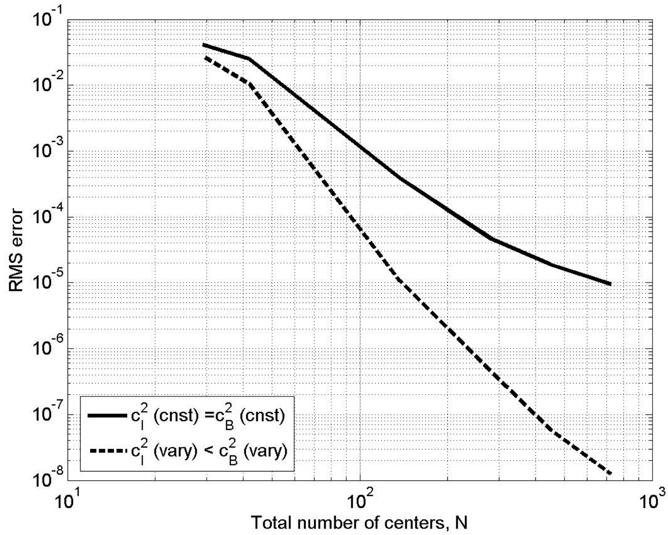

Figure 3: RMS errors for $\cos(2\pi[x+y])$ problem using the optimized β(N) for optimized constant c^2 and optimized variable $c^2_{\Omega\backslash\partial\Omega} << c^2_{\partial\Omega}$ as the number of data centers vary.

It was discovered by trial and error that a simple distribution of a variable c_j^2 for both the $\cos(2\pi[x+y])$ and the $\exp(2[x+y])$ problems could be obtained that dramatically reduced the RMS errors by using the following expression:

$$c_j^2 = \text{const}_1 * [1 + \text{const}_2 (-1)^j\ ], \tag{10}$$

where const_1= the optimal constant c^2(N) for the interior or boundary and $0.25 \leq \text{const}_2 \leq 0.65$. The parameter, const_2, determines the amplitude of the oscillations of const_1 as the index, j, varies from even and odd values. For both Poisson problems tested, it was observed that if $c^2(N)_{\Omega\backslash\partial\Omega} << c^2(N)_{\partial\Omega}$ the RMS errors dropped very fast with increasing N.

Figure 2 shows the variation of $(c_j^2)_{\Omega\backslash\partial\Omega}$ (*solid line*) and $(c_j^2)_{\partial\Omega}$ (*dotted line*), not to scale, for typical solutions of the two Poisson equations. The solid line is that of $(c_j^2)_{\Omega\backslash\partial\Omega}$ with the alternating values for even and odd numbered index, j. The dotted line is the distribution of $(c_j^2)_{\partial\Omega}$ with the alternating values for even and odd numbered index, j. For most problems tested, a recommended value of $(\text{const}_2)_{\partial\Omega}$ lies in the interval $0.49 \leq (\text{const}_2)_{\partial\Omega} \leq 0.55$, and the recommended value of $(\text{const}_2)_{\Omega\backslash\partial\Omega}$ lies in the interval, $0.25 \leq (\text{const}_2)_{\Omega\backslash\partial\Omega} \leq 0.33$.

Figure 3 shows the results of an optimization search for the best values of c_j^2 using $\text{const}_1 = c^2(N)_{\partial\Omega}$ and const_2 (dashed line) and the recalculated uniform c^2(N) (solid line) for the $\cos(2\pi[x+y])$ problem. Note that by simply allowing the set of c_j^2 to oscillate as well as be distinct on the boundary and interior has reduced the RMS errors by 3 orders of magnitude as N becomes increasingly larger.

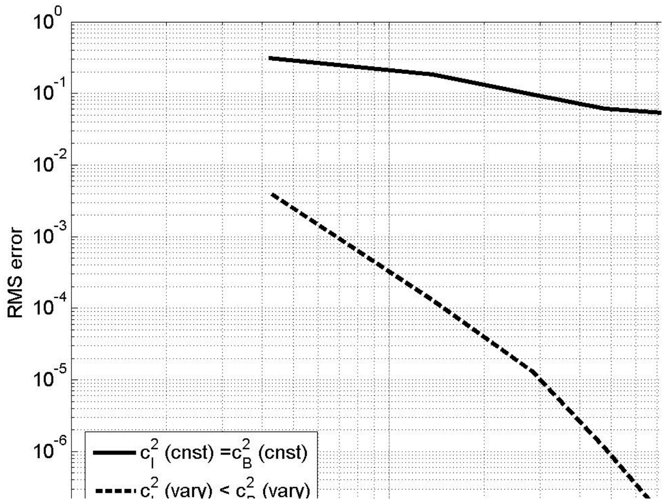

Figure 4: The RMS errors versus N for the exp(2[x+y]) problem with constant c^2 over Ω (*solid line*) and variable c_j^2 (*dashed line*).

Figure 4 shows a similar trend with the exponential elliptic problem that if $(c_j^2)_{\Omega\backslash\partial\Omega} << (c_j^2)_{\partial\Omega}$ and if the c_j^2 oscillate for odd and even index numbers, we obtain a dramatic reduction of RMS errors as the number of data centers, N increases.

3 High order time integration methods for parabolic partial differential equations

For diffusion parabolic PDEs, the operator $\mathcal{L}$ has the form:

$$\mathcal{L} = \frac{\partial}{\partial t} - \nabla \cdot (\kappa(\mathbf{x})\nabla), \tag{11}$$

where $\kappa(\mathbf{x})$ represents a diffusion coefficient that may have a spatial dependency.

From the initial conditions, one can find the initial set of expansion coefficients by solving

$$\mathbf{G}\chi(0) = U(\mathbf{x},0), \text{ where } \chi = [\alpha,\gamma]^T . \tag{12}$$

For time dependent PDEs, assume separation of variables such that the expansion coefficients, $\chi = \chi(t)$, are only functions of time and the RBFs are only functions of space. It is convenient to reorder all the points, $\{\mathbf{x}_j\}$, such that the first n_i points are associated with $\Omega\backslash\partial\Omega$, and the remaining n_b points are associated with $\partial\Omega$. This arrangement gives a convenient structure to the system of equations. Because the system of equations associated with $\frac{\partial U}{\partial t}$ on $\Omega\backslash\partial\Omega$ has the spatial portion related to the interpolation matrix, $\mathbf{G}$, but with a zero block matrix for those points associated with the boundaries, $\begin{matrix}\mathbf{G}_{\Omega\backslash\partial\Omega}\\ \mathbf{0}_{\partial\Omega}\end{matrix}$. Likewise, the spatial part of the parabolic PDE is a block matrix

$$\mathbf{H}\chi = \nabla \cdot (\kappa(\mathbf{x})\nabla)\mathbf{G}\chi = \mathbf{f} \text{ on } \Omega\backslash\partial\Omega \tag{13}$$

which has a similar structure to the **G** matrix, $\begin{matrix}\mathbf{H}_{\Omega\backslash\partial\Omega}\\ \mathbf{0}_{\partial\Omega}\end{matrix}$. The boundary conditions on $\partial\Omega$,

$$\text{ß}\mathbf{G}\chi = \mathbf{g} \text{ on } \partial\Omega \tag{14}$$

have the following structure, $\begin{matrix}\mathbf{0}_{\Omega\backslash\partial\Omega}\\ \mathbf{H}_{\partial\Omega}\end{matrix}$.

We can then express the time dependent PDE as a system of n_i ordinary differential equations in time plus n_b boundary constraint conditions as:

$$\begin{pmatrix} \mathbf{G}_{i,i} & \mathbf{G}_{i,b} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{bmatrix} \frac{d\chi_i}{dt} \\ \frac{d\chi_b}{dt} \end{bmatrix} - \begin{pmatrix} \mathbf{H}_{i,i} & \mathbf{H}_{i,b} \\ \mathbf{H}_{b,i} & \mathbf{H}_{b,b} \end{pmatrix} \begin{bmatrix} \chi_i \\ \chi_b \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \tag{15}$$

Notice that there no entries for the lower blocks of **G** since the boundary constraints are assumed to be constant in time.

Operating first on the rows of the boundary coefficients, χ_b, one obtains

$$\mathbf{H}_{b,b}^{-1}\mathbf{H}_{b,i}\,\chi_i + I_{b,b}\chi_b = \mathbf{H}_{b,b}^{-1}\mathbf{g} \tag{16}$$

With this relation, one can eliminate the block matrix, $\mathbf{H}_{i,b}$so the transformed **H** matrix is now in lower block form. Differentiating with time, and substituting $\frac{d\chi_b}{dt}$ we eliminate this term from the derivative of the time expansions, yielding:

$$(\mathbf{G}_{i,i}\text{-}\mathbf{G}_{i,b}\mathbf{H}_{b,b}^{-1}\mathbf{H}_{b,i})\frac{d\chi_i}{dt}\text{-}(\mathbf{H}_{i,i}\text{-}\mathbf{H}_{i,b}\mathbf{H}_{b,b}^{-1}\mathbf{H}_{b,i})\chi_i = (\mathbf{f}\text{-}\mathbf{H}_{i,b}\mathbf{H}_{b,b}^{-1}\mathbf{g}) \tag{17}$$

After obtaining the inverse of the matrix, $(\mathbf{G}_{i,i}\text{-}\mathbf{G}_{i,b}\mathbf{H}_{b,b}^{-1}\mathbf{H}_{b,i})$, this equation has the form:

$$\frac{d\chi_i}{dt}\text{-}\mathbf{\Lambda}\chi_i = \xi \tag{18}$$

The solution of this set of ordinary differential equations over $\Omega\backslash\partial\Omega$ has the form:

$$\chi_i(t) = \exp(-t\mathbf{\Lambda})\chi_i(0) + \mathbf{\Lambda}^{-1}\xi \tag{19}$$

where the exponential of a matrix is obtained by the Taylor series expansion, given by

$$\exp(-t\mathbf{\Lambda}) = \mathbf{I} + \frac{(-t\mathbf{\Lambda})}{1!} + \frac{(-t\mathbf{\Lambda})^2}{2!} + \frac{(-t\mathbf{\Lambda})^3}{3!} + \ldots \tag{20}$$

Once $\chi_i(t)$ is obtained, then the updated set of expansion coefficients for the boundary, χ_b is readily obtained. Second order time dependent wave equations can

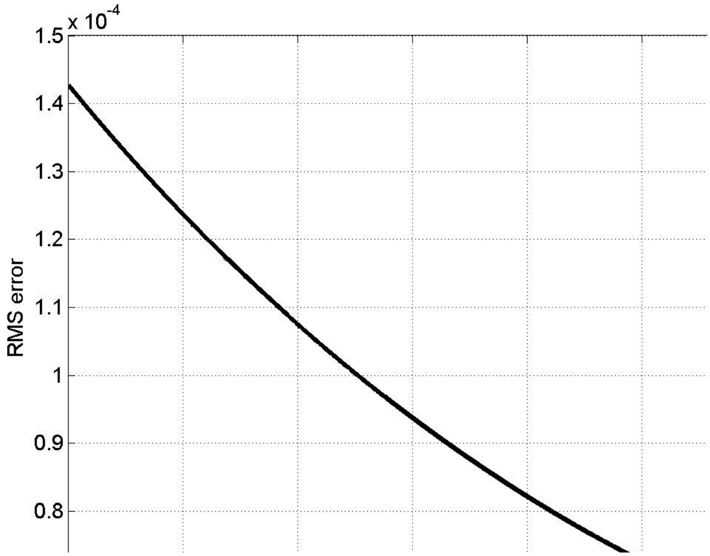

Figure 5: RMS errors for the time dependent two dimensional diffusion equation with the analytic integration method.

be solved by similar techniques. The time dependent solution will be sinusoidal for the expansion coefficients. The time dependent PDE problem over $\Omega\backslash\partial\Omega$ is cast into the method of lines with a set of n_b boundary constraint conditions over $\partial\Omega$.

This time integration approach was tested using the following two dimensional problem diffusion equation with $\kappa(\mathbf{x})$ =1 :

$$\frac{\partial \mathbf{U}}{\partial t} - \nabla^2\mathbf{U} = \mathbf{0}. \tag{21}$$

An exact solution of the above problem is:

$$\mathbf{U}(x,y,t)= e^{-t2\pi^2}\sin(\pi x)\sin(\pi y) \text{ over } \Omega = [0,1] \times [0,1] \tag{22}$$

with Dirichlet boundary conditions on all sides of $\partial\Omega$, and the initial conditions, $\mathbf{U}$(x,y,0).

The initial value problem was optimized for the best β and c_j^2 distributions on the boundary and interior. There were 137 total points, with 100 random points in $\Omega\backslash\partial\Omega$, and 37 on $\partial\Omega$. The time step was chosen to be a constant $\Delta t = 1{\cdot}10^{-5}$. Once exp($-\Delta t\mathbf{\Lambda}$) was formed, it was stored, and use to update $\chi(t)$.

Figure 5 shows the decrease of RMS errors for the test parabolic PDE problem. The initial value problem was interpolated onto a uniform 33x33 mesh and the RMS errors for the initial value were found to be $1.4{\cdot}10^{-4}$ for this problem with the chosen input parameters. For most applications, a problem with only 137 data centers can be consider to be a sparse problem. Because the exact solution is a decaying exponential in time, the numerical solution, U, decays rapidly in time , and likewise do the RMS errors as shown above.

4 Discussion

The objective of this study was to obtain the optimal numerical solution with a rather coarse discretization, rather than solving a problem with millions of discretization points that must be solved on massively supercomputers. This study shows the MQ-RBF can perform very well if modifications to the accepted MQ-RBF is undertaken. First, the exponent ,β should be a non-integer, and preferably above 5/2.

Second, it was observed that the $(c_j^2)_{\Omega\backslash\partial\Omega} << (c_j^2)_{\partial\Omega}$, and third, the c_j^2 should oscillate with the index, j with an average of about 1/2 about the mean. The study of the parameters is found in a recent paper by Wertz et al. [24]. It is also recommended that instead of using Gaussian elimination methods, the affine space decomposition method of Ling and Hon [23] . Finally, time dependent parabolic equations can be solved by analytic ordinary differential equation methods for high order accuracy.

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