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# Comparison of meshfree and mesh-based methods for boundary value problems in physics

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**Abstract.** Meshfree methods using basis expansion are common in computational physics, but their efficiency and accuracy depend on the quality of basis sets. We describe the application of radial basis functions (RBF), a class of basis functions attracting considerable interest and showing promising results. In the RBF approach, the solutions are interpolated over a chosen set of RBFs scattered over the domain. The value of a given RBF depends on the distance to the center, in contrast to the usual approach where the basis functions depend on the position. The advantage of the RBF method is that it can be efficient, simple to implement, and easily adaptable to irregular domains or higher dimensions. We study the application of this meshfree method to boundary value problems, including electrostatics and quantum systems. We show that the method is robust and flexible, and can be a compelling alternative to mesh-based methods.

## 1. Introduction

Computational modeling of physical systems often requires us to solve problems expressed in partial differential equations (PDE) such as the Laplace or Schrödinger equations. One family of numerical methods involves the discretization of space into regular grids or meshes. Common examples include the finite difference and finite element methods (FEM). Such mesh-based methods are direct and usually easy to use, except for irregular domains or high accuracy control. Nonetheless, they form a baseline for further improvement.

Another family of methods takes a meshfree approach. Rather than discretizing space, the solutions are approximated by a set of basis functions. Eigenfunction expansion is a familiar example. Recently, radial basis functions (RBF) have been shown to be good candidates for meshfree solutions.

We describe a meshfree RBF method in which the solutions are interpolated with a set of RBFs at scattered centers. We first discuss the interpolation of known functions in terms of RBFs to analyze general properties such as the size and shape of the RBF basis. We then apply the RBF method to solve PDEs such as the Poisson equation by collocation method which evaluates the differential operators at the RBF centers of the interpolant. The results show that the method is robust and flexible, and can be advantageous in comparison to mesh-based methods such as FEM in some cases, including scalability to higher dimensions.

## 2. Radial basis function interpolation

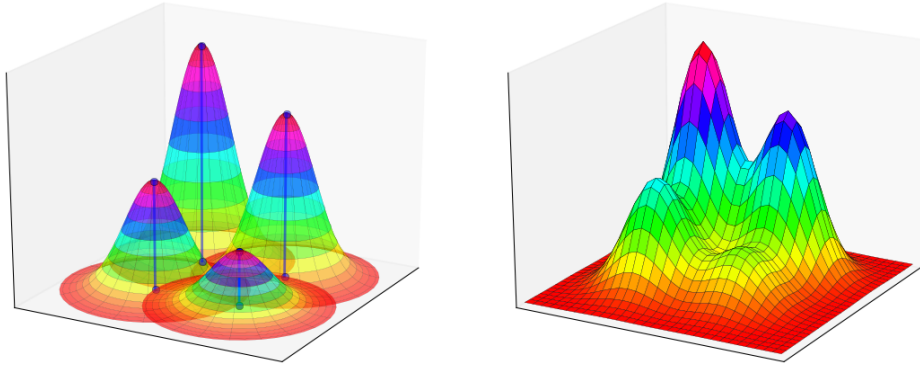
The basic idea of meshfree methods is scattered data interpolation [1, 2]. We assume that, like the FEM method [3, 4], the solution  $u$  can be approximated by expansion in a distance-based



RBF set  $\phi_i(\vec{r})$  as

$$u(\vec{r}) = \sum_{i=1}^N a_i \phi_i(\vec{r}). \quad (1)$$

where  $a_i$  are the expansion coefficients.



**Figure 1.** Scattered RBFs (left) and the resultant interpolation (right).

There are many possible functional forms for  $\phi_i$ . We list two commonly used RBFs as example, the Gaussian (GA) and the multiquadric (MQ),

$$\text{GA: } \phi_i(\vec{r}) = e^{-\epsilon^2 |\vec{r} - \vec{r}_i|^2}, \quad \text{MQ: } \phi_i(\vec{r}) = \sqrt{1 + \epsilon^2 |\vec{r} - \vec{r}_i|^2}, \quad (2)$$

where  $\epsilon$  is the shape (control) parameter, and  $\vec{r}_i$  are the nodes (centers) scattered over the domain of interest.

We can use Eq. (1) for scattered data interpolation (Fig. 1). For example, suppose we have four ( $N = 4$ ) known data points,  $u_i$  at  $\vec{r}_i$ ,  $i = 1$  to  $N$ . The scattered data points are not restricted to any particular geometry. The coefficients  $a_i$  can be determined by requiring

$$u(\vec{r}_i) = u_i, \quad (3)$$

where we have taken the nodes to coincide with the scattered data points. The result can be expressed as a matrix equation

$$\begin{bmatrix} \phi_1(\vec{r}_1) & \phi_2(\vec{r}_1) & \phi_3(\vec{r}_1) & \phi_4(\vec{r}_1) \\ \phi_1(\vec{r}_2) & \phi_2(\vec{r}_2) & \phi_3(\vec{r}_2) & \phi_4(\vec{r}_2) \\ \phi_1(\vec{r}_3) & \phi_2(\vec{r}_3) & \phi_3(\vec{r}_3) & \phi_4(\vec{r}_3) \\ \phi_1(\vec{r}_4) & \phi_2(\vec{r}_4) & \phi_3(\vec{r}_4) & \phi_4(\vec{r}_4) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}. \quad (4)$$

Eq. (4) can be solved for RBF expansion coefficients  $a_{1-4}$ . The matrix entries are defined at the RBF collocation points given by

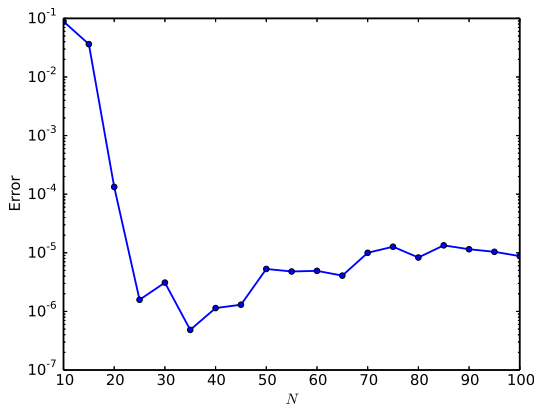
$$\phi_i(\vec{r}_j) = \phi(|\vec{r}_i - \vec{r}_j|) = \phi_j(\vec{r}_i), \quad (5)$$

where  $\phi$  is either a GA or MQ RBF in Eq. (2). Because the RBFs are based on the radial distance  $r_{ij} = |\vec{r}_i - \vec{r}_j|$  from the nodes, the system matrix is positive and definite. It can also be shown that the determinant is invariant under exchange of any pair of nodes because the scalar distances  $r_{ij}$  stay the same. Therefore, irrespective of node locations, the system matrix is well-conditioned, and the solution is assured to be nonsingular. In fact, the tent basis functions in 1D FEM are

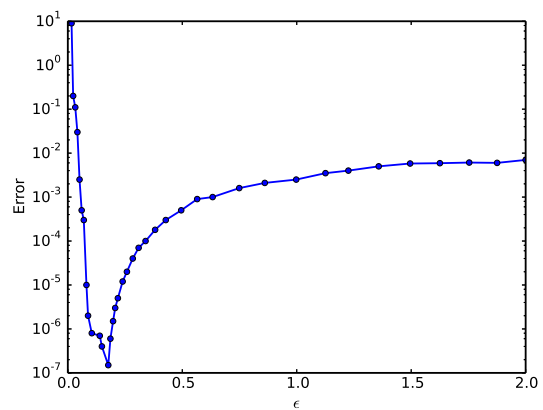
linear RBFs, and share some of above traits, except they are not infinitely differentiable like the GA or MQ. In general, however, if the basis functions were position (rather than distance) based, the above mentioned properties would no longer hold. In this respect, scattered data interpolation by RBFs has unique advantages.

Fig. 1 illustrates an example consisting of four Gaussian RBFs centered at the scattered data points. After obtaining the expansion coefficients  $a_{1-4}$  (vertical lines at the nodes in Fig. 1, left), the resultant interpolant Eq. (1) can be used to approximate the solution over the whole domain.

Specifically, we analyze RBF interpolation in terms of the number of RBFs,  $N$ , and the shape parameter  $\epsilon$  in a 1D test case. We use the test function  $u(x) = \exp(\sin \pi x)$ , with  $|x| \leq 1$ . For  $N$  nodes, we solve the  $N \times N$  linear system Eq. (4) with the GA RBFs.



**Figure 2.** Interpolation error as a function of  $N$ , the number (size) of the basis set, at a given shape parameter.



**Figure 3.** Interpolation error as a function of the shape parameter  $\epsilon$ , at a given basis size  $N$ .

In Fig. 2, we show the maximum absolute error (upper bound) in terms of the number of nodes,  $N$ , for a fixed shape parameter  $\epsilon = 1$ . For simplicity, the nodes are uniformly distributed in the interval  $x \in [-1, 1]$ . Initially, the error decreases rapidly with increasing  $N$ . Denser nodes result in more accurate representation as expected. However, after certain  $N \sim 40$ , the error remains flat, and accuracy does not improve. We see that there is a limit to the size of the basis set beyond which no benefit can be obtained.

We can also keep the size  $N$  constant and vary the shape parameter  $\epsilon$ . Fig. 3 displays the interpolation error as a function of  $\epsilon$  for a fixed  $N = 40$ . The error is large for both large and small values of  $\epsilon$ . There is an optimal shape parameter which minimizes the error,  $\epsilon \sim 0.2$  in this case. In general, the optimal  $\epsilon$  value depends on  $N$ . For best results, we need to find the best combination of  $N$  and  $\epsilon$  in practice.

### 3. RBF collocation method

The RBF collocation method is based on differentiating a RBF interpolant, from which the differentiation operator matrices can be built [5]. As an example, we use the collocation method to solve the 2D Poisson equation with the Gaussian RBF (equally applicable to 3D).

We consider a region surrounded by an arbitrary boundary (the domain). Let  $N$  be the total number scattered nodes. Of these, we assume the number of internal nodes is  $n$ , and the number of boundary nodes is  $N - n$ .

Substituting the interpolant Eq. (1) into the Poisson equation  $\nabla^2 u = f$ , we obtain

$$\nabla^2 u = \sum_i a_i \nabla^2 \phi_i(\vec{r}) = f(\vec{r}). \quad (6)$$

The collocation method, also known as Kansa's method [6], stipulates that the Poisson equation Eq. (6) be satisfied at the internal nodes  $\vec{r}_j, j \in [1, n]$ , and simultaneously, the boundary conditions be also satisfied at the boundary nodes  $\vec{r}_j, j \in [n+1, N]$ .

To be concrete, we assume Dirichlet boundary conditions. We have for the collocation method

$$\sum_i a_i \nabla^2 \phi_i(\vec{r})|_{\vec{r}=\vec{r}_j} = f(\vec{r}_j), \quad j = 1, 2, \dots, n, \quad (7a)$$

$$\sum_i a_i \phi_i(\vec{r}_j) = b_j, \quad j = n+1, n+2, \dots, N, \quad (7b)$$

where  $b_j$  are the potential values on the boundary. Casting Eq. (7a)–(7b) into matrix form we have

$$A\mathbf{a} = \mathbf{b}, \quad (8)$$

where  $\mathbf{a} = [a_1, a_2, \dots, a_N]^T$  is the column vector to be solved for, and

$$A = \begin{bmatrix} D_{11} & D_{12} & \cdots & D_{1N} \\ \vdots & \vdots & \vdots & \vdots \\ D_{n1} & D_{n2} & \cdots & D_{nN} \\ \phi_{n+1,1} & \phi_{n+1,2} & \cdots & \phi_{n+1,N} \\ \vdots & \vdots & \vdots & \vdots \\ \phi_{N1} & \phi_{N2} & \cdots & \phi_{NN} \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} f_1 \\ \vdots \\ f_n \\ b_{n+1} \\ \vdots \\ b_N \end{bmatrix}, \quad (9)$$

where  $f_j = f(\vec{r}_j)$  is the charge density at node  $j$ , and the differentiation operators and RBF values are defined as

$$D_{ij} = \nabla^2 \phi_i(\vec{r})|_{\vec{r}=\vec{r}_j} \equiv \nabla_j^2 \phi_i(\vec{r}_j), \quad \phi_{ij} \equiv \phi_i(\vec{r}_j). \quad (10)$$

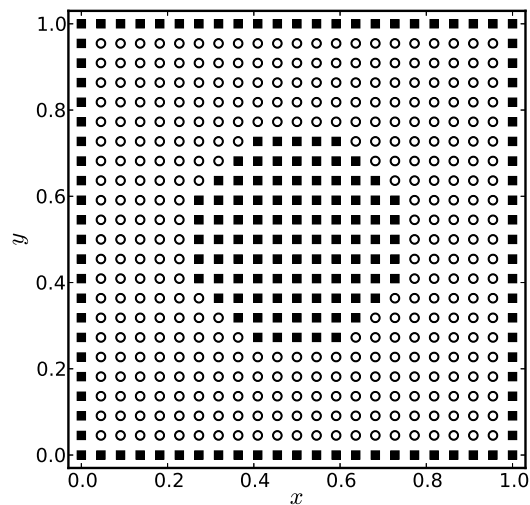
The system matrix  $A$  is square but asymmetric. It can be evaluated given the specific RBF (GA or MQ) and the nodes. If the operator is different than the Laplacian, it can be modified in a straightforward way. The vector  $\mathbf{b}$  consists of the charge densities  $f_j$  and the boundary values  $b_j$ . Once the necessary parameters are known, we can obtain the solutions  $\mathbf{a}$  by solving Eq. (8) with a standard matrix solver.

#### 4. Application and results

Let us apply the RBF collocation method to solve the special case of  $f = 0$  in Eq. (6) (Laplace equation) with Gaussian RBFs. The system geometry is a disk (roughly an octagon at the chosen spacing) in the center of a square box, Fig. 4. We assume the box is kept at zero potential and the disk at a constant potential (say 1). We simply distribute the nodes uniformly over the domain ( $23 \times 23$ ), though other choices are also possible, e.g., the Halton sequence. The number of internal nodes is  $n = 344$ , and the number of boundary nodes is  $N - n = 185$ . The  $\mathbf{b}$  vector Eq. (9) consists of zeros in the top  $n$  rows and ones in the bottom  $N - n$  rows.

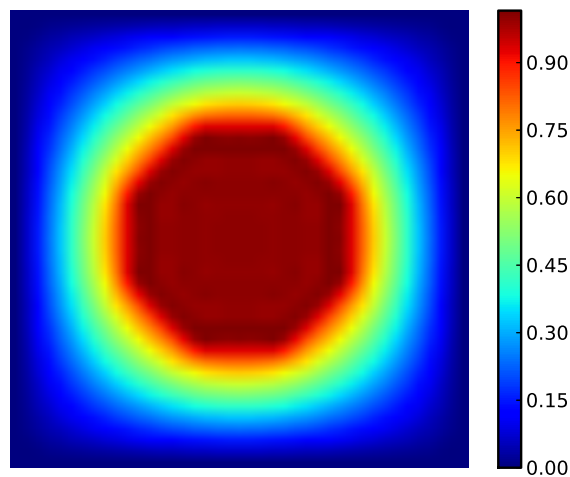
The basic differentiation operator is

$$\nabla^2 \phi_i(\vec{r}) = e^{-\epsilon^2 |\vec{r} - \vec{r}_i|^2} = 4\epsilon^2 e^{-\epsilon^2 |\vec{r} - \vec{r}_i|^2} (\epsilon^2 |\vec{r} - \vec{r}_i|^2 - 1). \quad (11)$$



**Figure 4.** The disk-in-a-box configuration. There are  $n = 344$  internal nodes ( $\circ$ ) and 185 boundary nodes ( $\blacksquare$ ) for a total of  $N = 529$  nodes. The potential is constant on the octagon and zero along the walls.

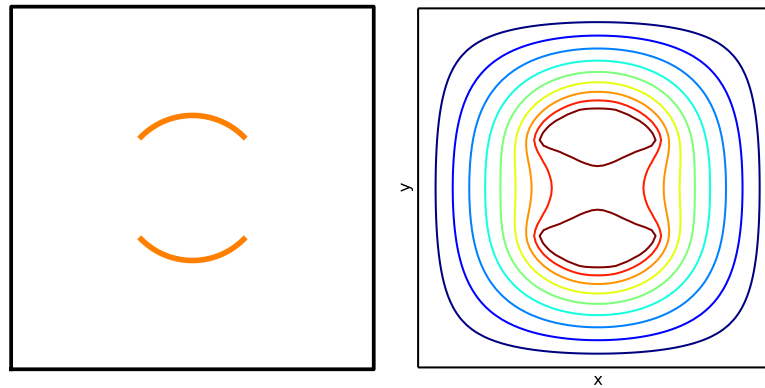
It can be readily evaluated to form the system matrix  $A$  given the nodes and the shape parameter  $\epsilon$ . As seen from Fig. 3, the value of  $\epsilon$  is critical to the accuracy and success of the RBF method. The accuracy depends on  $\epsilon$ , sometimes very sensitively, given the choice of RBF type and the placement of the nodes [7]. Typically, the extreme values, either very small or very large  $\epsilon$ , lead to very bad approximations. It is unknown, however, where the sweet spot is in general. Sometimes we must find it by trial and error (such as in Fig. 3 for the test function). From the applied physicists' perspective, we resort to physics to guide us. Suppose  $h$  is the typical distance between the nodes. We expect that the resolution should be such that  $\epsilon h \sim 1$ , or  $\epsilon \sim 1/h$ .



**Figure 5.** The potential for the disk-in-a-box configuration.

Fig. 5 shows the results of the RBF collocation method. The value  $\epsilon = 20$  is used (the actual spacing is  $1/22$ ). However, test shows that values from 10–25 works equally well. The potential is highest, and approximately constant, within the disk (or the octagon), and decreases to zero toward the walls as expected. It also shows correct symmetry from the configuration.

We also apply the collocation method to a different geometry in Fig. 6 consisting of two opposing circular arcs held constant potential inside a grounded box. It is much easier to



**Figure 6.** Circular arcs held at constant potential (left) and the potential contours (right).

distribute nodes along the arcs and in the domain with the RBF method than with a mesh-based method. The advantage to other irregular boundaries is evident.

Compared to FEM, the accuracy of the RBF method is good. Considering that sharp corners usually require higher density of nodes for the scattered data interpolation to be accurate, the RBF results with a modest number of uniform nodes in the present case are satisfactory. The RBF method is fast, and easier to use than FEM. The disadvantage is it is more difficult to control accuracy systematically.

With FEM, we can progressively reduce the error with smaller meshes (at least down to the limit before machine accuracy becomes a factor). In the RBF method, we expect that increasing the number of nodes will lead to more accurate results. However, if the number of nodes changes, we need to change the shape parameter accordingly, whose optimal value is not known a priori. And the situation may be different for different RBFs.

In summary, the meshfree RBF method can be an efficient method for problems involving PDEs. It is especially suitable for irregular boundaries and higher dimensions. For the case study with the Laplace equation, the RBF method performs equally well relative to mesh-based methods such as the FEM, but is easier to use. We are currently investigating the RBF method for other boundary value problems including quantum systems.

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### References

- [1] M. D. Buhmann, *Radial basis functions: theory and implementations*. (Cambridge University Press, Cambridge, 2003).
- [2] H. Wendland, *Scattered data approximation*. (Cambridge University Press, Cambridge), 2005.
- [3] J. N. Reddy, *An introduction to the finite element method*. (McGraw-Hill, New York), 1993.
- [4] J. Golde, J. Shertzer, and P. Oxley, Finite element solution of Laplaces equation for ion-atom chambers. *Am. J. Phys.*, **77**:81–86, (2009).
- [5] G. E. Fasshauer, *Meshfree approximation methods with MATLAB*. (World Scientific, Hackensack, NJ), 2007.
- [6] E. J. Kansa, Multiquadrics – a scattered data approximation scheme with applications to computational fluid dynamics II: Solutions to parabolic, hyperbolic, and elliptic partial differential equations. *Comp. Math. Appl.*, **19**:147–161, (1990).
- [7] E. Larsson and B. Fornberg, A numerical study of some radial basis function based solution methods for elliptic PDEs. *Comp. Math. Appl.*, **46**:891–902, (2003).