

Osculatory Interpolation in the Method of Fundamental Solution for Nonlinear Poisson Problems

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The Method of Fundamental Solution (also known as the F-Trefftz method or the singularity method) is an efficient numerical method for the solution of Laplace equation for both two- and three-dimensional problems. In recent years, the method has also been applied for the solution of Poisson equations by finding the particular solution to the nonhomogeneous terms. In general, approximate particular solutions are constructed using the interpolation of the nonhomogeneous terms by the radial basis functions. The method has been validated in recent papers. This paper presents an improvement of the solution procedure for such problems. The improvement is achieved by using radial basis functions called osculatory radial basis functions. Such functions make use of the normal gradient at boundary to obtain improved interpolation. The efficacy of the method is demonstrated for some prototypical nonlinear Poisson problems and for multiple Poisson equations. © 2001 Academic Press

Key Words: method of fundamental solutions; nonlinear Poisson problem; particular solution method; mesh free methods; radial basis functions; multiquadrics; osculatory interpolation; Hermite interpolation; diffusion–reaction equations; Liouville equation.

I. INTRODUCTION

The Poisson equation, $\nabla^2 u = f(x, u)$, where x is the position vector and u the dependent variable, is encountered in a variety of modeling situations in heat, momentum, and mass transfer, among others. Other examples of Poisson type of equations in computational physics include the Liouville equation, Chandrasekhar–Wares equation, Emden equation in astrophysics, geometry of conformal metrics, and so forth. The use of conventional

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numerical methods to solve such problems, viz., finite differences or finite elements, involve discretizing the entire domain of interest. For nonregular geometries, the process of element or grid generation and the associated bookkeeping of the elements and nodes can prove cumbersome and expensive in the user time and the CPU time, especially for three-dimensional (or higher) problems. Hence, in the past decade, there has been considerable interest to develop mesh-free methods to solve the nonlinear Poisson equation. Most common among these mesh-free methods is the dual-reciprocity boundary element method or DRBEM as an abbreviation (for example, 1–4). Here, the problem is reduced to the solution of the Laplace equation by finding approximate particular solutions to the nonhomogeneous terms. The Laplace equation, in turn, can be solved by a boundary-only discretization using the boundary element methods (BEM). The BEM, in turn, requires the evaluation of the singular integrals along the boundary. These singular integrations are easy to perform for two-dimensional problems but can be computationally expensive for the three-dimensional case. As an alternative, one can adopt a solution procedure called the *Method of Fundamental Solutions (MFS)* to solve the Laplace part of the problem. The MFS belongs to the general class of boundary collocation methods [5], and in this procedure, the solution is represented as a set of single layer potentials emanating from “source” points located outside the solution domain. The boundary conditions are satisfied by simple boundary collocation or a least square fitting of the boundary data. In this procedure, one avoids the problem of evaluation of the singular integrals needed in the boundary element method and in the dual-reciprocity methods. Hence, the procedure is computationally more efficient than the DRBEM. Some pertinent prior references on the MFS method are summarized in the following paragraph.

The Method of Fundamental Solutions (MFS) has been extensively applied for the solution of the linear partial differential equations. Some key references include the Laplace equation [6], the biharmonic equations [7], elasticity [8], fluid mechanics [9], and the linear diffusion reaction equations [10]. The method was also applied to the solution of nonhomogeneous linear Poisson equations (for example, $f = f(x)$) by combining the MFS with the particular solutions to the nonhomogeneous terms [11]. The particular solutions can be evaluated analytically for certain forms of the function, $f = f(x)$. More recently, the method has also been extended to solve a nonlinear Poisson problem (the thermal explosion problem) by Chen [12] using the approximate particular solutions and a simple Picard iteration to handle the iterations needed for the nonlinear terms. The solution scheme for nonlinear problems was improved by Balakrishnan and Ramachandran [13] who introduced the concept of a Matrix of Particular Solutions. Improved iterations with the direct Newton–Raphson method could be done by this approach and the applicability of the method to a large class of nonlinear Poisson problems was demonstrated [13]. These studies [12, 13] used the interpolation using the radial basis functions (RBF) for the representation of the Poisson terms and for the evaluation of the particular solution. The RBF interpolation uses only the function values at chosen points in the domain called as the knots or the centers. Additional information on the values of the normal gradient at the boundary is available or needs to be computed in most cases as the part of the solution for these classes of problems. The RBF approximation can be improved by using these information on the normal gradients. This concept was introduced by Ramachandran and Karur [14] in the context of the dual-reciprocity boundary element method, and the basis functions which also fit the boundary values of the normal gradients were referred to as the osculatory radial basis functions (ORBF). The concept can be viewed as an extension of the familiar spline fitting

or the Hermite interpolation commonly used in one-dimensional data fitting. The ORBFs provide additional degrees of freedom, thereby permitting a more accurate interpolation for the same number of interior knots. The purpose of the present paper is to demonstrate the ORBF interpolation in the context of the MFS for nonlinear Poisson problems and to document the improvements in the solution as a result of using this approach. The layout of the paper is as follows. In Section II, a brief synopsis of the Method of Fundamental Solutions for nonlinear Poisson problems is presented in order to provide the necessary background. In Section III, we present the concept of osculatory interpolation and its implementation in the method of fundamental solution. Results for nonlinear Poisson problems with uniform and mixed boundary conditions are presented in Section IV, and the concluding Section V summarizes the key findings.

II. THE PARTICULAR SOLUTION METHOD

Consider the Poisson equation, to be solved over a domain Ω in \mathbb{R}^2 or \mathbb{R}^3 with enclosing boundary Γ ,

$$\nabla^2 u = f(x, y, z, u) \quad \text{in } \Omega \quad (1)$$

with the following mixed boundary conditions imposed over the boundary Γ , Dirichlet:

$$u = \bar{u} \quad \text{over } \Gamma_1 \quad (2a)$$

Neumann:

$$\frac{\partial u}{\partial n} = p = \bar{p} \quad \text{over } \Gamma_2, \quad (2b)$$

where $\Gamma_1 + \Gamma_2 = \Gamma$ and the bar denotes prescribed values.

Also, the more general case of Robin boundary conditions can also be considered with,

$$\frac{\partial u}{\partial n} + hu = -hu_o \quad \text{over } \Gamma_2, \quad (2c)$$

where h is the heat/mass transfer coefficient, and u_o is the prescribed value of u of the surroundings. This boundary condition needs only minor modifications to the solution scheme.

In the method of particular solutions, the solution is expressed as the sum of the homogeneous problem with a set of modified boundary conditions and a particular solution which satisfies no specific boundary conditions, i.e.,

$$u = v + w, \quad (3)$$

where the function v satisfies the Laplace equation,

$$\nabla^2 v = 0 \quad \text{in } \Omega, \quad (4)$$

and the function w is a particular solution defined as the solution to

$$\nabla^2 w = f \quad \text{in } \Omega. \quad (5)$$

Thus, the problem is solved by using two separate approximations for v and w as suggested by Eq. (3). The solution to the homogeneous part, v , can be obtained by the method of fundamental solutions. Here v is expressed as,

$$v = \sum_{i=1}^{nb} a_i G_i, \quad (6)$$

where G_i is the fundamental solution to the Laplace equation with the pole or source located at a point i (which is outside the domain under consideration). The coefficients a_i are found by boundary collocation, i.e., making Eq. (6) satisfy the (modified) boundary condition on the variable v at nb number of boundary points. The fundamental solutions G_i are standard and are given as follows: For three-dimensional problems, $G_i = r_i^{-1}$ corresponding to the source point i , where r_i is the Euclidean distance from the source (or pole) i . Similarly, $G_i = -\ln r_i$ for two-dimensional problems.

A slight modification is needed for two-dimensional problems. Here, the a constant term is needed in the expansion as pointed out by Golberg and Chen [11]. Hence, the number of source points is taken as one less than the number of boundary collocation points and the solution for v is represented as

$$v = a_o + \sum_{i=1}^{nb-1} a_i G_i. \quad (6a)$$

The next part of the approximation is to evaluate the particular solution, w . In order to do this, the forcing function f is approximated over Ω using suitable basis functions. For irregular geometry, the radial basis functions (RBF) have proven to be most versatile for interpolation at scattered data points. A number of different types of RBFs have been used in the context of solution of partial differential equations [15–21]. These include linear distance functions, thin plate splines, multiquadrics, and RBFs with compact supports. In general, the interpolation of the nonhomogeneous term f in terms of a set of RBF functions ϕ_k can be defined as

$$f = \sum_{k=1}^{nt} \alpha_k \phi_k, \quad (7)$$

where α_k are a set of expansion coefficients obtained by interpolating at a total of nt nodes in accordance to the following equation

$$f_j = \sum_{k=1}^{nt} \phi_{jk} \alpha_k \quad j = 1, 2, \dots, nt, \quad (8)$$

where ϕ_{jk} is the function ϕ_k evaluated at any point j . The corresponding matrix denoted as $\tilde{\Phi}$ is also known as the interpolation matrix.

Equation (8) can be expressed in vector–matrix form,

$$\vec{f} = \tilde{\Phi} \vec{\alpha} \quad \text{or} \quad \vec{\alpha} = \tilde{\Phi}^{-1} \vec{f}, \quad (9)$$

which provides the conditions needed for the calculation of the expansion constants, α_k . The particular solution, w which satisfies Eq. (5), is obtained from the particular solutions

to each of the ϕ_k functions, and can be expressed as

$$w = \sum_{k=1}^{nt} \alpha_k \psi_k, \quad (10)$$

where ψ_k is given by

$$\nabla^2 \psi_k = \phi_k. \quad (11)$$

The explicit analytical forms for ψ_k can be evaluated for various types of RBF ϕ_k . This makes the computation of the approximate particular solutions a simple task.

Now, since the solution $u = v + w$ for computational efficiency, the two parts of the solution can be combined, and the composite solution can be expressed as

$$u = \sum_{i=1}^{nb} a_i G_i + \sum_{k=1}^{nt} \alpha_k \psi_k. \quad (13)$$

Using the inverse transformation in Eq. (9) and collocating at all the (nt) points one can rewrite this equation in vector form as

$$\vec{u} = \tilde{G} \vec{a} + \tilde{\Psi} \tilde{\Phi}^{-1} \vec{f} \quad (14)$$

or

$$\vec{u} = \tilde{G} \vec{a} + \tilde{\beta} \vec{f}, \quad (15)$$

where $\beta = \tilde{\Psi} \tilde{\Phi}^{-1}$ is called the Matrix of Particular Solutions. Equation (15) is then the compact approximate analytical representation of the solution. The matrices \tilde{G} and $\tilde{\Psi}$ are defined in an analogous manner as the matrix $\tilde{\Phi}$.

For a Dirichlet problem, one chooses nb collocation points on the boundary Γ and $nt-nb$ interior points and nb (note $nb-1$ in 2D) source points outside the boundary. The boundary conditions are substituted into Eq. (15) and the equations are rearranged and solved for the unknowns. These unknowns are the boundary fitting coefficient vector, \vec{a} , and the value of the variable u at the interior points. The resulting equations are nonlinear if f is a nonlinear function of u and are solved by a modified Newton–Raphson iteration. If at certain boundary points, the Neumann conditions are specified, then Eq. (15) is differentiated to obtain an expression for $\partial u / \partial n$. The known value of $\partial u / \partial n$ is substituted for these points, and the set of equations are correspondingly augmented since the value of u is also an unknown at this point. More details of the method can be found in [13]. We now proceed to the discussion of osculatory interpolation and its implementation in the above formulation.

III. OSCULATORY INTERPOLATION FOR PARTICULAR SOLUTIONS

Ramachandran and Karur [14] introduced the concept of osculatory interpolation using radial basis function. Here the interpolation of the function f is carried out using not only the nodal values of the dependent variable but also the normal gradient at the boundaries. This

requires nb additional degrees of freedom for satisfying the slope conditions at the nb boundary points. The interpolating equations for the forcing function f is now written as

$$f = \sum_{k=1}^{nt} \alpha_k \phi_k + \sum_{k=1}^{nb} \delta_k \varphi_k, \quad (16)$$

where the additional set of interpolating functions φ_k , which are linearly independent of ϕ_k , are introduced, and δ_k are the corresponding additional interpolating coefficients. The linear independence between the two functions ϕ_k and φ_k is needed since both the interpolating and osculating conditions are applied at the same boundary point. The resulting matrices are found to be nonsingular if the two functions are chosen as linearly independent. The osculatory interpolation is also known as the Hermite interpolation. The theory of Hermite interpolation using RBF is however not well established and only limited studies appear to have been published [22–24]. In these studies, the osculatory and interpolatory conditions are applied at different points and hence two separate sets of functions are not required. More theoretical basis for Hermite interpolation and, in particular, the invertability of the coefficient matrix (the matrix appearing in Eq. 19 later in the text) should be examined in future studies. In this paper we demonstrate the use of this method only by computational experiments and not on a functional analysis framework.

The coefficients α_k and δ_k are in Eq. (16) computed using both interpolation and osculation conditions as discussed below. At all the interpolating nodes (boundary and interior), we set $f = f_i$, the nodal value of the forcing function, i.e.,

$$f_i = \sum_{k=1}^{nt} \phi_{ik} \alpha_k + \sum_{k=1}^{nb} \varphi_{ik} \delta_k \quad (i = 1, 2, \dots, nt). \quad (17)$$

At all the nb boundary points, the additional osculation conditions are imposed, i.e.,

$$\left. \frac{\partial f}{\partial n} \right|_i = \sum_{k=1}^{nt} \left(\frac{\partial \phi_k}{\partial n} \right)_i \alpha_k + \sum_{k=1}^{nb} \left(\frac{\partial \varphi_k}{\partial n} \right)_i \delta_k \quad (i = 1, 2, \dots, nb). \quad (18)$$

The equations can be setup in matrix form as shown below in Eq. (19) and the coefficients α_k and δ_k are given by Eq. (20):

$$\begin{pmatrix} \bar{f} \\ \bar{f}' \end{pmatrix} = \begin{pmatrix} \tilde{\phi} & \tilde{\varphi} \\ \tilde{\phi}' & \tilde{\varphi}' \end{pmatrix} \begin{pmatrix} \bar{\alpha} \\ \bar{\delta} \end{pmatrix} \quad (19)$$

$$\begin{pmatrix} \bar{\alpha} \\ \bar{\delta} \end{pmatrix} = \begin{pmatrix} \tilde{\phi} & \tilde{\varphi} \\ \tilde{\phi}' & \tilde{\varphi}' \end{pmatrix}^{-1} \begin{pmatrix} \bar{f} \\ \bar{f}' \end{pmatrix}. \quad (20)$$

This gives us the requisite coefficients for the interpolation scheme. Note that in the above equations the symbol $'$ represents the normal derivative at the boundary points.

The particular solutions for the osculation interpolation can be defined in terms of two functions, ψ , η , satisfying

$$\nabla^2 \psi_k = \phi_k \quad (21)$$

$$\nabla^2 \eta_k = \varphi_k. \quad (22)$$

The solution to the problem u is now given by,

$$u = \sum_{i=1}^{nb} a_i G_i + \sum_{k=1}^{nt} \psi_k \alpha_k + \sum_{k=1}^{nb} \eta_k \delta_k, \quad (23)$$

and the normal gradient p is given by

$$p = \frac{\partial u}{\partial n} = \sum_{i=1}^{nb} a_i \frac{\partial G_i}{\partial n} + \sum_{k=1}^{nt} \frac{\partial \psi_k}{\partial n} \alpha_k + \sum_{k=1}^{nb} \frac{\partial \eta_k}{\partial n} \delta_k. \quad (24)$$

Substituting for α_k and δ_k from Eq. (20), we get the required collocation equations,

$$\begin{pmatrix} \bar{u} \\ \bar{p} \end{pmatrix} = \begin{bmatrix} \tilde{G} \\ \tilde{G}' \end{bmatrix} \bar{a} + \begin{bmatrix} \tilde{\psi} & \tilde{\eta} \\ \tilde{\psi}' & \tilde{\eta}' \end{bmatrix} \begin{pmatrix} \tilde{\phi} & \tilde{\varphi} \\ \tilde{\phi}' & \tilde{\varphi}' \end{pmatrix}^{-1} \begin{pmatrix} \tilde{f} \\ \tilde{f}' \end{pmatrix}. \quad (25)$$

Equation (25) is now the representation of the solution when using the ORBF for constructing the particular solution and now replaces Eq. (15). Note that the function values at all points (boundary + interior) and the normal gradients at the boundary points are now included in the computation.

For solution purposes, the nonlinear term f is expressed in a quasilinear form, $k_1 + k_2 u$, where, the

$$k_1 = f(u_m) - u_m \left. \frac{df}{du} \right|_{u_m}$$

$$k_2 = \left. \frac{df}{du} \right|_{u_m},$$

where u_m is the value of u at the current level of iteration. The linearized form is substituted into Eq. (25) and the system of linear equations is solved iteratively to convergence. More details of the procedure can be found in Ramachandran and Karur, [14]. The procedure is similar to a Newton–Raphson method. For any given problem, the equations for the nt nodal values of u and nb normal gradients at the boundary are assembled and solved for the unknown coefficients a_i and the unspecified boundary values of u and fluxes p and in addition the $(nt-nb)$ interior values of u . Note that the boundary gradients (at the Dirichlet points) are directly calculated as a part of the solution and not in a postprocessing scheme unlike the earlier method. The test cases and results for a few prototypical problems will now be discussed in the next section.

The solution accuracy often depends on the choice of the RBFs. A number of papers have addressed this issue but there is no clear consensus on the choice of the functions. Multiquadrics have been used for many applications and was used in our earlier study with unaugmented RBFs [13]. However, the results are often sensitive to the choice of the shift parameter. Hence, we used the thin plate splines and the cubic function as the RBFs here. These functions are defined below:

Thin plate spline: $\phi_i = r^2 \log(r)$

Cubic: $\varphi_i = r^3$

The corresponding particular solutions are as follows:

Particular solutions for the cubic RBF (r^3)

$$\eta_i = \frac{r^5}{25}$$

Particular solutions for Thin Plate Splines ($r^2 \log r$)

$$\psi_i = \frac{r^4 \log r}{16} - \frac{r^4}{32}$$

Other choices of RBFs could also be made and often the choice is dependent on the nature of the function being interpolated. A recent study [25] indicates that cubic function and higher order TPS may be a reasonable choice for a wide range of problems. Also, the use of compactly supported RBFs is also being used [26] and these functions could also be used for the interpolation. Further studies should address these issues.

IV. TEST CASES AND RESULTS

In this section we demonstrate the efficacy of the solution procedure discussed earlier in Section III for some typical problems. The governing equation is chosen as: a power law form: $f(u) = M^2 u^n$ for test case 1, and more complex kinetic rate forms are examined in case 2. Uniform Dirichlet boundary conditions are used for these cases. The solution procedure for a mixed boundary conditions is tested in Case 3 for a power law rate form. Case 4 shows the application of the method to a system of differential equations. In these test cases, a simple circular geometry is used, and this geometry is sufficiently representative to demonstrate the grid free nature of the method. However, in order to show the application for a more irregular geometry, the case of a trilobe catalyst is considered in test case #5.

For test cases 1 to 4, the circle radius is chosen as 1.0 and the 16 boundary nodes, and 60 interior nodes were used as the base case for the discretization. The location of the nodes is shown in Fig. 1. The number of boundary nodes were increased to 32 for a finer set of collocation points, and the internal nodes were also correspondingly increased to 120. These results on a finer set of nodes were used to demonstrate the discretization errors and the convergence of the method. The finer mesh used is shown schematically in Fig. 2.

The source points were placed on a circle of radius 1.4 in a uniform manner. The source radius was also varied in order to test the effect of this parameter of the solution. It was found, in general, that the results are not sensitive to the source radius within a wide range of 1.4 to 5.0.

Case 1: Power Law form: Dirichlet Conditions

The function $f(u) = M^2 u^n$ is used in cases 1 and 3. Here, the parameter, M , is called the Thiele modulus in chemical engineering literature and represents the ratio of kinetic to transport resistances in the domain. The larger the Thiele modulus, the steeper the profiles of the dependent variable, and for very large Thiele moduli, a boundary layer with a thickness of the order of $(1/M)$ is present. In such cases, traditional methods, such as finite elements, require a fine discretization of the region near the boundary layer for increased accuracy. Here we demonstrate that even a coarse mesh can provide reasonably accurate results when oscillatory interpolation is used.

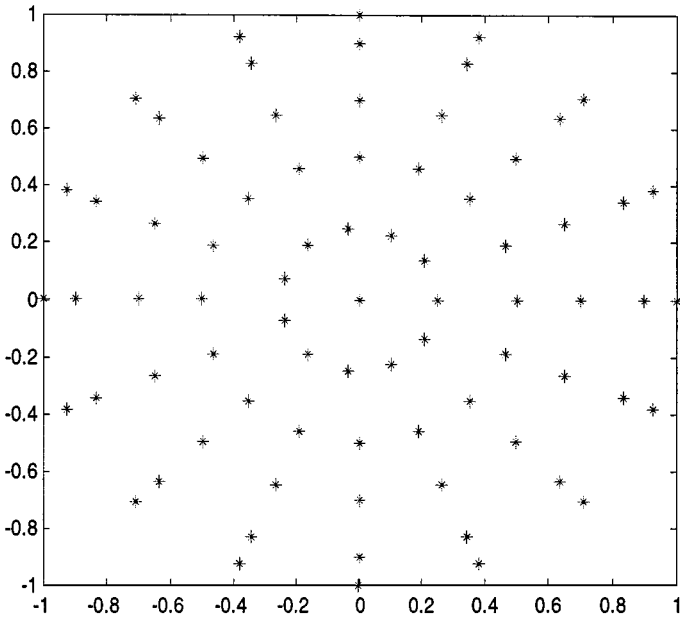


FIG. 1. Coarse node placement for the circle.

Case 1a: Power Law: first order case ($n = 1$)

We first consider a first-order reaction ($n = 1$) with Dirichlet boundary conditions for which case an analytical solution is available, viz.,

$$u = \frac{I_0(Mr)}{I_0(M)} \quad \text{in } \Omega \quad (27)$$

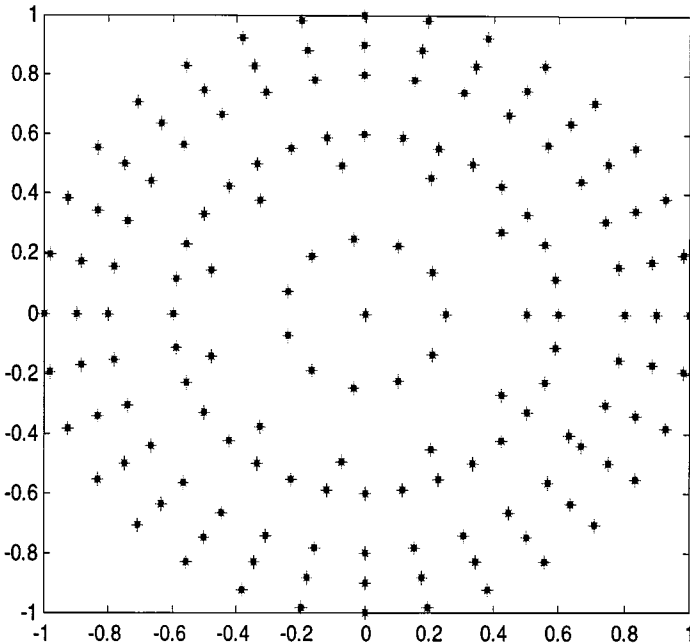


FIG. 2. Fine node placement for the circle.

TABLE I
Solution for $n = 1, M = 100$; Comparison of Accuracy
of Numerical Results

Location r	Concentration Profiles			TPS Coarse Set
	Coarse Set	Fine Set	Analytical	No Osculation
0.9	0.3936	0.3895	0.3884	0.3853
0.7	0.0714	0.0621	0.0599	0.0662
0.5	0.0112	0.0094	0.0097	0.0111
0.25	0.0014	4.26×10^{-4}	0.0017	0.0019
0.0	5×10^{-4}	2×10^{-4}	3.55×10^{-4}	1.35×10^{-4}
Gradient at $x = 1$	9.5634	9.4935	9.486	9.6596

$$\frac{\partial u}{\partial n} = \frac{M I_1(Mr)}{I_0(M)} \quad \text{on } \Gamma. \quad (28)$$

The comparison of the solutions are shown in Table I along with those without osculatory interpolation using TPS. As one can see, the gradient values using osculatory interpolation are more accurate than with traditional RBF interpolation. The concentration values are also shown in Table I and compared with an analytical solution. The source points in this case were placed on a circle center (0, 0) and radius 1.4. The source radius was also varied in order to test the effect of this parameter of the solution. It was found that the results are not sensitive to the source radius as indicated earlier in the text.

Case 1b: Power Law: Second order reaction ($n = 2$)

The case of second-order reaction ($n = 2$) is considered next and the results are presented in Table II. Here the solution is compared with the numerical solution by a 1-D code BEM1D (Ramachandran, [2]) which is considered to be very accurate for comparison purposes. It is seen that both the concentration profiles and the fluxes are close to the BEM1D solution. The use of regular TPS without osculation predicted the same concentration profiles but predicted the flux with an error of about 6%. This shows some advantage of using the osculatory

TABLE II
Results for a Second-order ($n = 2$) Reaction, $M = 100$

X	Coarse Set	Fine Set	BEM1D Values	TPS Coarse Set
	Concentration Values			No Osculation
0.90	0.5486	0.5289	0.5235	0.5230
0.70	0.2713	0.2480	0.2260	0.2494
0.50	0.1458	0.1258	0.1335	0.1423
0.25	0.0962	0.0783	0.0916	0.0991
0.00	0.0800	0.0689	0.0803	0.0846
Gradient at $x = 1$	7.8564	7.7264	7.7525	8.1459

TABLE III
Solutions for Exponential and Substrate Inhibited Rate forms;
Dirichlet Conditions

Rate form → Locations	Liouville equation $f = 5 \exp(-u)$	Thermal explosion $f = -\exp(u - 1)$	Substrate inhibition $f = 1040u/(1 + 50u + 1000u^2)$
u at $r = 0.9$	0.8589	1.0568	0.9438
u at $r = 0.7$	0.5964	1.1559	0.8445
u at $r = 0.0$	0.1127	1.3176	0.6796
p at $r = 1.0$	1.4332	-0.5900	0.5821

interpolation. In most problems, the information on the boundary gradients is needed and the method proposed here calculates these quantities directly as part of the solution.

Case 2: Dirichlet Conditions: Complex Rate Models

The computer program was also tested for various nonlinear rate forms which are some prototypical problems in physics and engineering. Results for the following three cases are presented in Table III. For all cases, the source points were on a circle center (0, 0) radius 1.4 and the node placements shown in Fig. 1 were used in the computations. The parameter values were chosen so that comparison with other numerical method could be done.

Case 2.1: Liouville equation. Here the rate function is chosen as

$$f = \frac{\lambda^2}{8} \exp(-u). \quad (29)$$

This equation is encountered in many physical situations. Here, $\lambda^2 = 40$ was used for numerical studies. The results shown in Table III were compared to an earlier study by Liao and Zhu [27] and the agreement was verified.

Case 2.2: Thermal explosion problem:

$$f = -\exp(u - 1). \quad (30)$$

This represents a situation with an exponentially increasing thermal source in a confined space and the solution to this problem is needed for a safe design of combustion and other exothermic processes. The numerical results are in agreement with other computed results.

Case 3: Substrate inhibition kinetics:

$$f(u) = M^2 u / (1 + \alpha u + \beta u^2). \quad (31)$$

This problem is a representation of enzyme catalyzed biochemical reaction. The parameters chosen were $M^2 = 1040$, $\alpha = 50$, and $\beta = 1000$, and the problem has multiple steady states here. The results shown in Table IV reproduced one of the steady states accurately. Bifurcation studies using this method in combination with programs for continuation and bifurcation analysis such as AUTO [28] can be done to check if all the steady states are

TABLE IV
Gradient and Concentration Values along the Boundary
for Test Case #3, $n = 2$, $M = 100$

Angular Location	Fine Set	Coarse Set
<i>Case 1: Gradient Values</i>		
0.0982	5.198	
0.1963	4.4186 ^a	4.5046
0.2945	3.6392	
0.4909	3.7296	
0.589	3.7042 ^a	3.5598
0.6872	3.6787	
<i>Case 2: Concentration Values</i>		
1.669	0.4534	
1.7671	0.3589 ^a	0.3557
1.8653	0.2644	
2.0617	0.2022	
2.1598	0.1899 ^a	0.1807
2.258	0.1775	

^a Interpolated values.

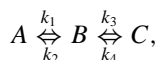
predicted by this numerical scheme. We have not performed such studies and the more detailed bifurcation analysis are considered outside the theme of this paper.

Case 3: Mixed Boundary Conditions

Case 3 demonstrates the application of the method for a nonlinear forcing function of the power law type ($n = 2$) with Dirichlet and Neumann boundary conditions imposed over various parts of the perimeter. Here is a unit circle considered with Dirichlet conditions ($u = 1$) are imposed over the first and third quadrants and Neumann conditions ($p = 0$) are imposed over the rest of the perimeter. It is to be noted that at the junction of the Dirichlet and Neumann boundaries, the flux is undefined and increases rapidly and is singular at the junction. Representative profiles of u for a Thiele modulus of 5.0 are shown for the geometry of a circle in Fig. 3 for the mixed boundary conditions. The profiles qualitatively agree with those expected and agree well with other solution methods. To determine the convergence of the scheme, the results are presented for both the coarse and fine set of collocation points in Table IV. The solutions calculated by these two sets of nodes are fairly close to each other, indicating the convergence of the procedure. As a further test, solutions were also evaluated at interior noncollocation points and compared to each other. The mean square error over 71 interior noncollocation points was 0.006 and 2.5×10^{-5} between the two successive refinements, which is indicative of the convergence of the scheme.

Case 4: Multiple Differential Equations

To illustrate the efficacy of the procedure for a system of nonlinear equations, we consider the hypothetical reaction scheme,



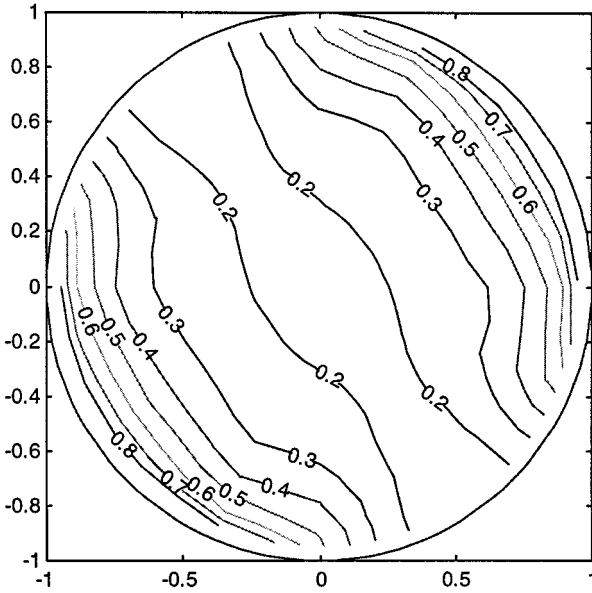


FIG. 3. Concentration profiles for a second order reaction $f = 25u^2$ with mixed boundary conditions (Case 3).

where the reversible reactions between A and B are assumed to be second order and the reaction from B to C is assumed to be first order. The governing equations for the independent species A , B , and C (designated as 1, 2, and 3) are given by

$$\nabla^2 u_1 = k_1 u_1^2 - k_2 u_2^2 \quad (32)$$

$$\nabla^2 u_2 = k_3 u_2 + k_2 u_2^2 - k_1 u_1^2 - k_4 u_3 \quad (33)$$

$$\nabla^2 u_3 = k_4 u_3 - k_3 u_2. \quad (34)$$

The values of the constants for a chosen simulation were $k_1 = 5.0$, $k_2 = 1.0$, $k_3 = 5.0$, and $k_4 = 3.0$ and the results are shown in Table V. The solution procedure adopted was to solve the individual diffusion reaction equations sequentially, with a Newton–Raphson iteration for each variable. An initial guess for u_2 is used to start of the solution of the equation for A , and the values of u_1 , u_2 , u_3 are updated with each iteration until convergence is obtained (change in sum of the squared error $\sim 1e-9$). It may be noted here that the sequential solution procedure used may not be the best method for the multiple set of algebraic equations and may not converge in all cases. More efficient convergence schemes can be used but our objective here was to see how the particular solution method works for a system of differential equations. This has not been done in any of the earlier studies. The results indicated that the method is equally accurate for multiple differential equations of the Poisson type. The approximate particular solution for each individual reactions are dependent on each other but this coupling appears to produce no spurious numerical problems.

Case 5: Nonregular Geometries

In this case, we demonstrate the efficacy of the method for solving nonlinear problems in nonregular domains. We consider the example of a trilobe, shown in Fig. 4. In the simulation

TABLE V
Results of Multiple Reactions (Case 4) with Mixed (D-N)
Boundary Conditions as in Case 3

Boundary Values	A	B	C
p at $\theta = 0$	1.5645	-0.2398	-1.3248
p at $\theta = \pi/8$	1.1123	-0.2337	-0.8786
C at $(0,0)$	0.5743	1.0034	1.4223

studies, only a third of the trilobe is interpolated in view of the symmetry of the domain. It may be noted that splitting the domain into one third does not eliminate the singularity at the cusp but is merely a convenience for keeping the number of knots small. The two cases we consider are as follows:

(i) Dirichlet—concentration of 1.0 all over the perimeter, (Fig. 5)

(ii) Dirichlet–Neumann—concentration of 1.0 over some part of the perimeter and no flux over the remainder of the perimeter. (Figure 5, with Neumann conditions imposed from point A to point B)

The source points were located at distance of 0.3 from each boundary collocation point. The concentration profiles for each case with a value of $M = 3.0$ for a second-order reaction are shown in Figs. 6 and 7, which agree qualitatively with those expected.

This study illustrates a case where the geometry is complex and the results demonstrate that the procedure works well for this case thus indicating the usefulness of the method.

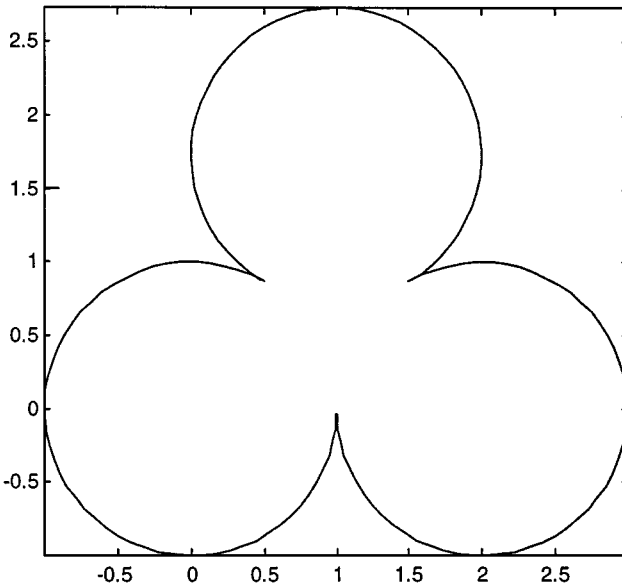


FIG. 4. Illustration of a nonregular geometry—a trilobe (Case 5).

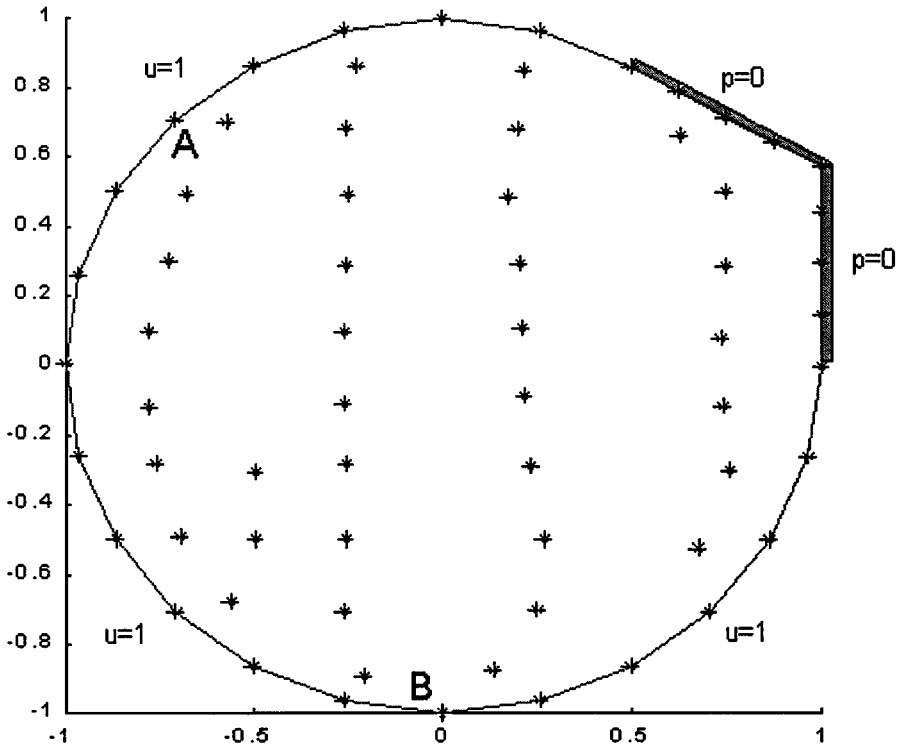


FIG. 5. Node placement and boundary conditions on a cusp of the trilobe for the case when Dirichlet boundary conditions are imposed all over the surface of the trilobe.

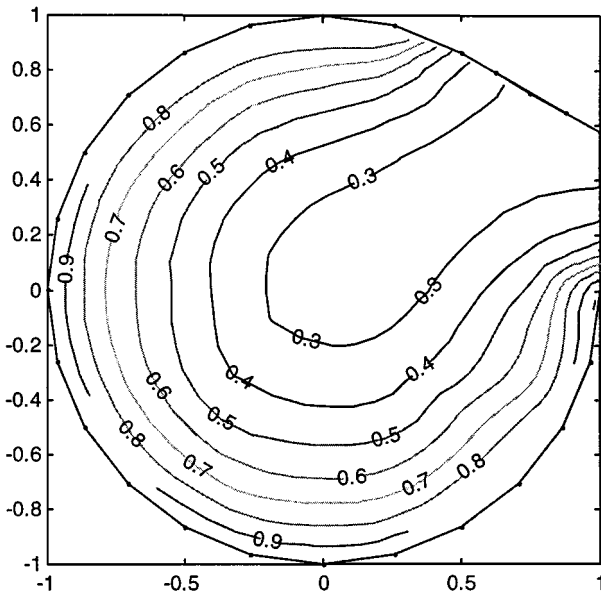


FIG. 6. Concentration profiles for a trilobe with Dirichlet boundary conditions (one cusp shown) for a second order reaction ($f = 9u^2$).

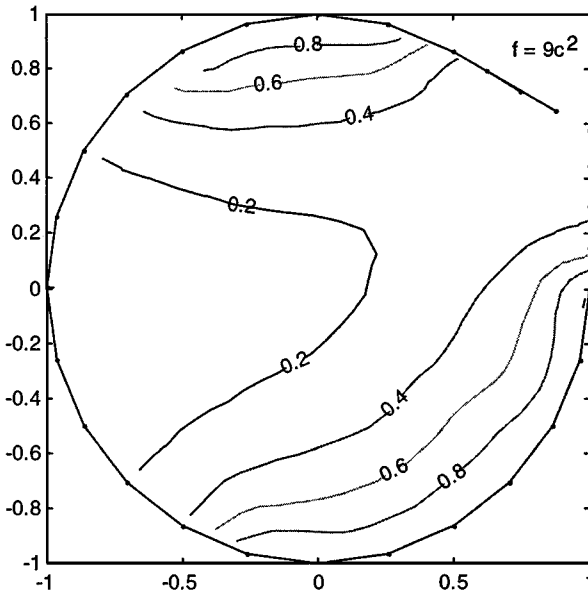


FIG. 7. Concentration profiles for a trilobe with mixed boundary conditions (one cusp shown) for a second order reaction ($f = 9u^2$).

V. CONCLUSIONS AND SUMMARY

In this paper, we present an extension of a grid-free solution technique, called the Method of Fundamental Solutions, for solving nonlinear Poisson problems. The solution method presented here uses a set of nodes in the interior in order to interpolate the function values. It may be noted that this interpolation is needed only for the purpose of obtaining an approximate particular solution. Thus, there is no need to approximate any differential operators (second derivatives for the problem presented here) in the interior, and hence one source of error associated with the finite difference and finite elements is eliminated. Further, the nodes can be distributed in any order in the interior and no special bookkeeping or tracking of inter-element continuity is needed, another advantage of the method. Once the particular solution is obtained, the problem is reduced to a boundary collocation problem. This problem is solved by choosing a set of boundary collocation nodes and a corresponding set of source nodes which are placed outside the domain of solution. The set of collocation equations are then written for all the function values at the internal and boundary nodes as well as for the normal gradients at the boundary collocation points. One of the improvements in this paper is that the normal gradient values are also included in the interpolation of the function which is then referred to as the osculatory or Hermite interpolation. The osculation is similar to a spline fitting and permits the function to take the correct slope at each of the boundary collocation points. This increases the accuracy of the solution. The accuracy has been demonstrated for a number of test problems. The test problems include systems with a complex geometry and a case of mixed boundary conditions. Further, the method has been applied for the first time for the solution a system of differential equations, and the results are satisfactory. For the solution of problems with larger complex domain, the method can be easily used in conjunction with the domain decomposition. The domain decomposition will be very effective here since many of the matrix coefficients (associated

with, for example, the matrix of a particular solution) can be used in various subdomains. Further, although the results presented in this paper are for two-dimensional problems, the method is directly applicable to 3-D or even higher dimensions. The only changes are in the expressions for the fundamental solution and for the form of the particular solution, as indicated in the text. Thus, the computer programs for implementing the method is independent of the dimensionality of the problem which is a unique feature of this method. The method is also easy to implement in the context of multinode iterative schemes. Here the particular solution can be extrapolated from the coarse node level to the fine node level. Thus, corrections at the finer node levels can be done only on the boundary collocation points which requires a solution of a smaller set of linear algebraic equations. In view of the many advantage, the use of the method presented in this paper to a variety of important application problems can be expected in the future.

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