A comparison between Lagrange multiplier and penalty methods for setting boundary conditions in mesh-free methods

Comparación de los metodos de multiplicadores de Lagrange y penalizacion para aplicar condiciones de frontera en métodos sin malla

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***Resumen* — Una simulación de una viga en voladizo se llevó a cabo con el objetivo de comparar los resultados de dos Métodos sin malla, Element Free Galerkin y el Método de Interpolación usando Funciones de Base Radial, utilizando dos métodos diferentes para imponer las condiciones de frontera esenciales. Los resultados fueron validados con la solución analítica del problema, obtenida por Timoshenko en [20]. Fue posible concluir que ambos métodos muestran un buen desempeño para la solución del problema simulado. Sin embargo, algunas consideraciones se deben tener en cuenta cuando dichos métodos se vayan a usar en otro tipo de aproximaciones en las que no es posible aplicar fácilmente las condiciones de contorno esenciales.**

***Palabras Clave* — Imposición de Condiciones de Frontera de Dirichlet, Método de Penalización, Método de Multiplicadores de Lagrange.**

***Abstract* — A simulation of a cantilever beam was carried out with the aim of comparing the performance of two mesh-free methods: element-free Galerkin and radial point interpolation methods. In this implementation, we use two different methods to set boundary conditions. The results were compared with the analytical solution of the cantilever problem using Timoshenko formulation [20]. In the paper, we demonstrate that both numerical methods are accurate compared to the analytical solution. However, some consideration must be taken into account when applying these methods to more complex simulations that cannot be well approximated by the boundary conditions scheme.**

***Keywords* — Setting Boundary Condition, Penalty Method, Lagrange Multiplier Method**

I. INTRODUCTION

One of the most important advances in the field of numerical methods was the development of the Finite Element Method (FEM) in the 50's [10]. The method has been shown to be useful for modeling numerous complex problems in applied mechanics and related fields and is very well established in current engineering practice. Among the most outstanding weakness of FEM is that it relies on meshes or elements that are connected together by nodes with a strict topology. For this reason, it is very difficult to create an accurate and high-quality mesh to solve complex problems. Even with modern meshing software, this task is difficult and is not always possible to be performed automatically without human intervention. For example, it is very difficult to simulate needle insertion or crack growth in materials with arbitrary and complex paths as the topology between the nodes must be modified at every iterations. Also, considerable accuracy is lost when handling large deformation as the energy function becomes non-linear [11]. Mesh-Free methods (MFree) were introduced with the objective of solving some of those issues and to be more adaptable to difficult problems. The main advantage of MFree methods is that the simulation is built from nodes only [18] and do not require strict topology constraints between the node as with FEM.

As with FEM methods, MFree methods represent an alternative solution to the weak-form of differential equations that model practical engineering problems for which neither the strong-form solution, nor the exact solution can be computed.

Some of the early MFree methods were the vortex method [7] and the finite differences method with arbitrary grids [13]. Another well-known MFree method is the Smoothed Particle Hydrodynamics (SPH) [15] method introduced to model astrophysical phenomenon such as exploding stars and dust clouds with no boundaries.

According to the nomenclature made by Liu in [10], MFree methods can be classified in three main categories based on its formulation: based on weak forms, based on collocation, and based on a combination of these two formulations. For the weak form formulation, the Element Free Galerkin Method (EFGM) proposed by Belytschko [8] [4] made significant contributions in developing, improving, and popularizing MFree methods for mechanical problems. In fact, new MFree methods such as Radial Point Interpolation Method (RPIM) were developed by Liu, et al in [16] from Belytschko's work.

A variation of Belytscho's method is the local Petrov-Galerkin method proposed by Alturi [2] and the local radial point interpolation method proposed by Liu [14]. These last methods are known as *local weak form methods* as they only solve the weak-form equation in small quadrature domains over the general domain. Some other MFree weak-form methods have been proposed, such as the hp-cloud method [Arm96], the partition of unity finite element method [3], the finite spheres method [9], the free-mesh method [21], and many more.

Despite the advantages of MFree methods over the FEM, MFree techniques are still under development and much attention has been given to overcome some of their limitations. For instance, when solving boundary value problems, the imposition of the boundary conditions may be a problem since some of the MFree shape functions do not always satisfies the Kronecker-delta condition. This makes the imposition of boundary conditions more complicated than its FEM counterpart. Several methods have been proposed to set boundary conditions including: Lagrange multipliers method [4], the penalty method [22] [6], modified variational principle method [19], the coupling of FEM and EFGM [5], singular weight functions for MLS method [17]. While all of these techniques are workable, only some of them have the simplicity of FEM.

The aim of this study is to compare the performance of two MFree methods, EFGM and RPIM, as well as to evaluate their performance when the boundary conditions are set with the penalty or the Lagrange multipliers methods. Numerical studies have been performed for a cantilever beam which is often used for benchmarking numerical methods, as the exact analytical solution is known.

In the following sections, a brief overview of the two MFree method implemented is presented. Then, the formulation of how to set the boundary condition is summarized. The results of the simulations are presented in Section V, and finally we conclude in the last section.

II. A BRIEF OVERVIEW OF MESH-FREE METHODS

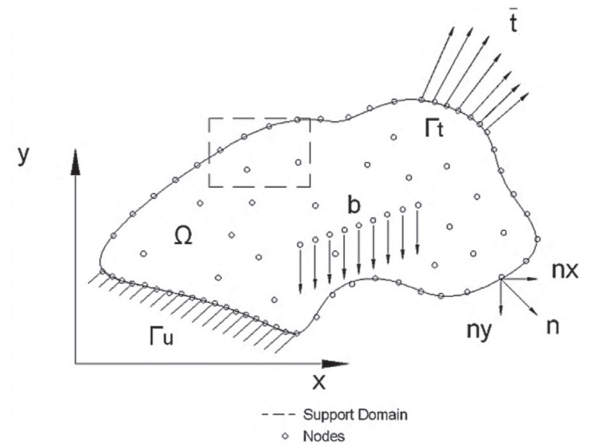

Figure 1: Two dimensional continuum solid [12]

For two dimensional problems, it is assumed that the geometry of the domain is independent of the z-axis, and all the external loads and forces are independent in the z-coordinate, and are applied only in the x-y plane. A 2-D graph of the problem is shown in Figure 1. The system of equation for a 2-D stationary isotropic material is given as follows:

Equilibrium Equation:	$\boldsymbol{L^T\sigma + b = 0}, \quad in\, \Omega,$	(1)
Natural boundary condition:	$\boldsymbol{\sigma n} = \bar{t}, \quad in\, \Gamma_i,$	(2)
Essential boundary condition:	$\boldsymbol{u} = \bar{\boldsymbol{u}}, \quad in\, \Gamma_u,$	(3)

where $\boldsymbol{L}$ is a differential operator of size 3 x 2, $\boldsymbol{\sigma}$ is the stress tensor of size 3 x1, $\boldsymbol{u}$ is the displacement vector of size 2 x1, $\boldsymbol{b}$ is the body force vector of size 2 x 1, $\bar{\boldsymbol{t}}$ is a scalar representing the prescribed traction, $\bar{\boldsymbol{u}}$ is a vector of size 2 x 1 and is the material displacement, and $\boldsymbol{n}$ is the normal vector of size 2 x 1 facing outward. The last three variables are considered on the boundary. The standard variational (weak) form of the system of equations given by Equations (1) to (3) and is solved [11] by the following equation:

$$\int_\Omega (\boldsymbol{L\delta u})^T(\boldsymbol{DLu})d\Omega - \int_\Omega \boldsymbol{\delta u^T b}d\Omega - \int_\Gamma \boldsymbol{\delta u^T}\bar{t}d\Gamma = \boldsymbol{0},$$

(4)

where $\boldsymbol{D}$ is the matrix of elastic constants of size 3 x 3 using the Young's modulus and Poisson ratio as parameters, see [12] for more detail.

Because a mesh topology is not used in MFree methods, the field variable (component of displacement) $\boldsymbol{u}$ at any point $\boldsymbol{p} = (x,y)$ within the problem domain is interpolated using the displacement at its nodes within the support domain Ω of the point at $\boldsymbol{p}$, as follows:

$$\boldsymbol{u}(\boldsymbol{p}) = \sum_{i=1}^{n} \phi_i(\boldsymbol{p})\boldsymbol{u}_i = \boldsymbol{\Phi}(\boldsymbol{p})\boldsymbol{U}_s, \quad (5)$$

where n is the number of nodes in a small local support domain around the point at $\boldsymbol{p}$, $\boldsymbol{u}_i$ is the nodal field variable at the *ith*-node, $\boldsymbol{U}_s$ is a vector of size n x 2 that collects all the field variables at these nodes, and $\boldsymbol{\Phi}(\boldsymbol{p}) = \{\phi_i(\boldsymbol{p}) | i = 1 \text{ to } n\}$ is the shape function of the *ith*-node determined using the nodes that are included in the small local support domain around $\boldsymbol{p}$. A number of ways to construct shape functions have been proposed. In our work, we discussed two of the most widely used methods, the RPIM and the MLS approximations.

Radial Point Interpolation Shape Function

The radial point interpolation augmented with polynomials can be written as:

$$\boldsymbol{u}^h(\boldsymbol{p}) = \sum_{i=1}^{n} R_i(\boldsymbol{p})a_i + \sum_{j=1}^{m} s_j(\boldsymbol{p})b_j, \quad (6)$$

$$R_i(\boldsymbol{p}) = (r_i^2 + (a_c d_c)^2)^q, \qquad a_c < 0, \quad (7)$$

$$\boldsymbol{s}^T(\boldsymbol{p}) = \{1\ x\ y\ x^2\ xy\ y^2\}, \quad \boldsymbol{m} = \boldsymbol{6}, \quad (8)$$

where $R_i(\boldsymbol{p})$ is known as the multi-quadratic radial function, n is the number of nodes into the support domain, $\boldsymbol{s}$ is vector of size 6 x 1 corresponding to the polynomial basis function in the space coordinates, and m is the number of monomials. The coefficients a_i and b_j are constants to be determined, the parameters a_c, d_c and q in Equation 7 are dimensionless shape parameters, and r_i is the distance between each node couples. In this study, a quadrature support domain is used to select the nodes that will be part of the approximation.

After some algebraic manipulations (see [10] for details), Equation 6, can be re-written in terms of the radial point interpolation shape function and the nodal parameter $\boldsymbol{u}$, as:

$$\boldsymbol{u}(\boldsymbol{p}) = \{\boldsymbol{R}^T(\boldsymbol{p})\boldsymbol{s}^T(\boldsymbol{p})\}\boldsymbol{G}^{-1}\boldsymbol{U}_S, \quad (9)$$

where, $\boldsymbol{\Phi}^{\mathbf{T}}(\mathbf{p}) = \{\mathbf{R}^{\mathbf{T}}(\mathbf{p})\, \mathbf{s}^{\mathbf{T}}(\mathbf{p})\}\mathbf{G}^{-1}$. (10)

Moving Least Square Interpolation Shape Function

The Moving Least Square (MLS) approximation is defined as:

$$\boldsymbol{u}^h(\boldsymbol{p}) = \sum_{j=1}^{m} \boldsymbol{s}_j(\boldsymbol{p})\boldsymbol{a}_i(\boldsymbol{p}) = \boldsymbol{s}^T(\boldsymbol{p})\boldsymbol{a}(\boldsymbol{p}), \quad (11)$$

$$\boldsymbol{a}^T = \{a_1(\boldsymbol{p}) \quad a_2(\boldsymbol{p}) \ldots \quad a_m(\boldsymbol{p})\}, \quad (12)$$

where $\boldsymbol{s}(\boldsymbol{p})$ is defined the same way as in Equation 8, and $\boldsymbol{a}(\boldsymbol{p})$ is a coefficient vector of size m x 1 given by Equation 12. After some algebraic manipulation, Equation 11 can be re-written in terms of the shape function $\boldsymbol{\Phi}(\boldsymbol{p})$ and the nodal parameter $\boldsymbol{u}$, as below;

$$\boldsymbol{u}(\boldsymbol{p}) = \boldsymbol{s}^T(\boldsymbol{p})\boldsymbol{A}^{-1}(\boldsymbol{p})\boldsymbol{B}(\boldsymbol{p})\boldsymbol{U}_S, \quad (13)$$

where, $\boldsymbol{\Phi}^T(\boldsymbol{p}) = \{\boldsymbol{s}^T(\boldsymbol{p})\boldsymbol{A}^{-1}(\boldsymbol{p})\boldsymbol{B}(\boldsymbol{p})\}$. (14)

A and **B** are matrices of size 3 x 3 determined by:

$$\boldsymbol{A}(\boldsymbol{p}) = \begin{bmatrix} \sum_{i=1}^{n} W_i & \sum_{i=1}^{n} x_i W_i & \sum_{i=1}^{n} y_i W_i \\ \sum_{i=1}^{n} x_i W_i & \sum_{i=1}^{n} x_i^2 W_i & \sum_{i=1}^{n} x_i y_i W_i \\ \sum_{i=1}^{n} y_i W_i & \sum_{i=1}^{n} x_i y_i W_i & \sum_{i=1}^{n} y_i^2 W_i \end{bmatrix} \quad (15),$$

$$\boldsymbol{B}(\boldsymbol{p}) = \begin{bmatrix} W_1 & W_2 & \ldots & W_n \\ x_1 W_1 & x_2 W_2 & \ldots & x_n W_n \\ y_1 W_1 & y_2 W_2 & \ldots & y_n W_n \end{bmatrix} \quad (16)$$

where W($\mathbf{p}$) is the cubic spline function and has the following form of:

$$W(\boldsymbol{p}) = \begin{cases} \frac{2}{3} - 4\bar{r}_i^2 + 4\bar{r}_i^3 & \bar{r}_i \le 0.5 \\ \frac{4}{3} - 4\bar{r}_i + 4\bar{r}_i^2 - \frac{4}{3}\bar{r}_i^3 & 0.5 < \bar{r}_i \le 1 \\ 0 & \bar{r}_i > 1 \end{cases} \quad (17)$$

$r_i = \frac{|p - p_i|}{r_w}$, and r_w is the size of the support domain (18)

III. SETTING BOUNDARY CONDITION FOR MESH-FREE METHOD

As mentioned previously, some of the MFree methods still have the difficulty to easily set the boundary conditions because most of the MFree shape functions, constructed from moving least square approximation, do not satisfy the Kronecker delta property. In the present work, we evaluate two different methods to specify boundary conditions in 2-D. Below, we present the mathematical formulation of both penalty and the Lagrange multipliers methods.

Penalty Method

The penalty method is a convenient alternative to specify the essential boundary conditions, in which the diagonal element of the stiffness matrix is:

$$\boldsymbol{K}_{ii} = \alpha \boldsymbol{K}_{ii}, \quad (19)$$

where, α is the penalty coefficient that is much larger number than the components of the stiffness matrix $\boldsymbol{K}$ of size 3 x 3. Usually for FEM α is determined as:

$$\alpha = 10^4 \sim 10^8 \times (\boldsymbol{K}_{ii})_{max} \tag{20}$$

Therefore, the constrained variational weak form (Equation 4) using the penalty method is the following:

$$\int_{\Omega} (\boldsymbol{L}\delta\boldsymbol{u})^T(\boldsymbol{DLu})d\Omega - \int_{\Omega} \delta\boldsymbol{u}^T\boldsymbol{b}d\Omega - \int_{\Gamma_t} \delta\boldsymbol{u}^T\bar{t}d\Gamma - \delta\int_{\Gamma_u} \frac{1}{2}(\boldsymbol{u}-\bar{\boldsymbol{u}})^T\alpha(\boldsymbol{u}-\bar{\boldsymbol{u}})d\Gamma = \boldsymbol{0}, \tag{21}$$

Lagrange Multipliers Method

In this method, the function to specify the boundary conditions is written in an integral form using the Lagrange multiplier $\boldsymbol{\lambda}$,

$$\int_{\Gamma_u} \boldsymbol{\lambda}^T((\boldsymbol{u}-\bar{\boldsymbol{u}})d\boldsymbol{\Gamma}. \tag{22}$$

Therefore, the weak form Equation 4 can be re-written as:

$$\int_{\Omega} (\boldsymbol{L}\delta\boldsymbol{u})^T(\boldsymbol{DLu})d\boldsymbol{\Omega} - \int_{\Omega} \delta\boldsymbol{u}^T\boldsymbol{b}d\boldsymbol{\Omega} - \int_{\Gamma_t} \delta\boldsymbol{u}^T\bar{\boldsymbol{t}}d\boldsymbol{\Gamma} - \int_{\Gamma_u} \delta\boldsymbol{\lambda}^T(\boldsymbol{u}-\bar{\boldsymbol{u}})d\boldsymbol{\Gamma} - \int_{\Gamma_u} \delta\boldsymbol{u}^T\boldsymbol{\lambda}d\boldsymbol{\Gamma} = \boldsymbol{0}, \tag{23}$$

where, $\boldsymbol{\lambda}$ is the Lagrange multipliers matrix, which are unknown functions of the coordinates and can be written in the following nodal matrix form:

$$\boldsymbol{\lambda} = \sum_{I}^{n_\lambda} \begin{bmatrix} \boldsymbol{N_I} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{N_I} \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda_{UI}} \\ \boldsymbol{\lambda_{VI}} \end{bmatrix} \tag{24}$$

$$\boldsymbol{N_k^n(s)} = \frac{(\boldsymbol{s}-\boldsymbol{s_0})(\boldsymbol{s}-\boldsymbol{s_1})\ldots(\boldsymbol{s}-\boldsymbol{s_{k-1}})(\boldsymbol{s}-\boldsymbol{s_{k+1}})\ldots(\boldsymbol{s}-\boldsymbol{s_n})}{(\boldsymbol{s_k}-\boldsymbol{s_0})(\boldsymbol{s_k}-\boldsymbol{s_1})\ldots(\boldsymbol{s_k}-\boldsymbol{s_{k-1}})(\boldsymbol{s_k}-\boldsymbol{s_{k+1}})\ldots(\boldsymbol{s_k}-\boldsymbol{n})} \tag{25}$$

$N_k^n(s)$ are the Lagrange interpolants used in the conventional FEM.

IV. NUMERICAL SIMULATION

A cantilever beam of size 4.8 m x 1.2 m was discretized by a cloud of points with 175 nodes, and the cells background by 55 nodes as shown in Figure 2. A force of 10x10[5] N in -y direction was applied at the end of the beam. A Young modulus of 200 x10[9] and a Poisson ratio of 0.26 was used to define material properties (A36 structural steel). As for the parameters of the shape functions, we define a quadrature support domain with 0.7 m and the shape parameters for RBF as $a_c=2$ and $q=1.03$. In the MLS approximation, a polynomial basis function of second order was used (m =3).

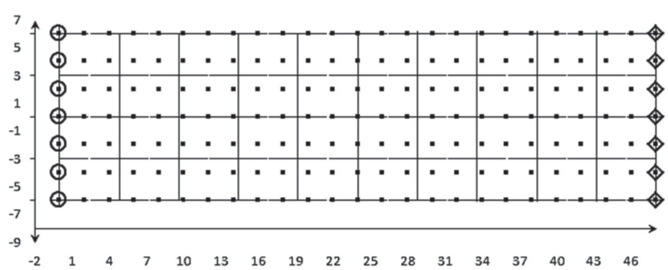

Figure 2: Discretized Cloud of Point for the Cantilever Beam

The exact solution for a cantilever beam was formulated in [20] and is expressed by:

$$\text{Strain}\begin{cases} u_x = -\dfrac{P}{6EI}\left[(6L-3x)x + (2+v)\left[y^2 - \dfrac{D^2}{4}\right]\right] & (26) \\ u_y = \dfrac{P}{6EI}\left[3vy^2(L-x) + (4+5v)\dfrac{D^2x}{4} + (3L-x)x^2\right] & (27) \end{cases}$$

Stress

$$\sigma_{xx} = -\frac{P(L-x)y}{I} \quad (28)$$

$$\sigma_{yy} = 0 \quad (29)$$

$$\tau_{xy} = \frac{P}{2I}\left[\frac{D^2}{4} - y^2\right] \quad (30)$$

where E and v are the Young's modulus and Poisson ratio respectively, and I is the moment of inertia of the body. The other parameters are geometric dimensions as illustrated in Figure 3.

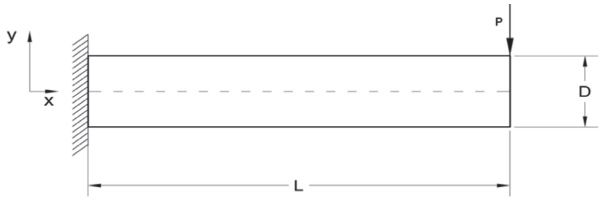

Figure 3: Cantilever Beam Subjected to a Force P at the End

V. RESULTS

The deflection of the beam u_x of the middle plane, y=0, computed with the MFree methods is shown in Figure 4. A total of 4 curves were obtained, the combination of every MFree method implemented with every method to set the boundary conditions. The differences for all the numerical methods relative to the analytical solution are in the order of 10^{-6} millimeter. Figure 5 shows the absolute error between the MFree methods and the exact solution for better comparison. Additionally, the values of the shear stress for the cross section of the beam in x = L/2 can be seen in Figure 6.

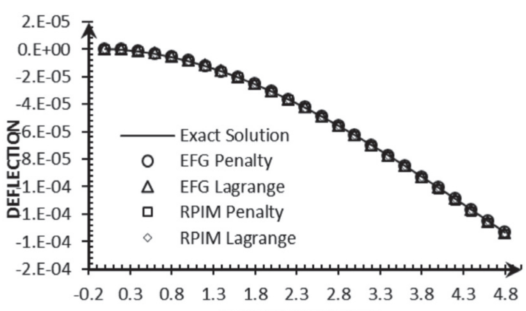

Figure 4: Deflection u_x at y=0

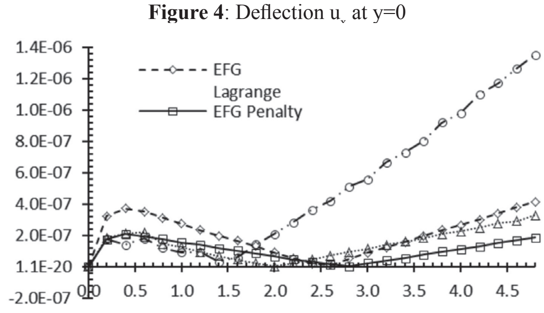

Figure 5: Absolute Error.

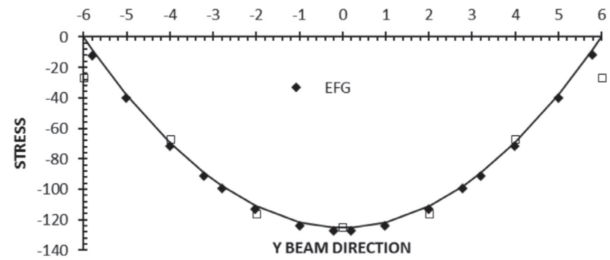

Figure 6 Shear Stress Distribution on the Cross-section x = 2.4 meters.

VI. CONCLUSION

MFree methods represent a good alternative to simulate mechanical problems such as beam deformation. Excellent simulation results were obtained by combining two different MFree methods (EFG and RPIM) and two different methods to set the boundary conditions. As one can see in Figure 4, the deflection of the beam in the middle plane is very accurate for all simulations (the absolute error is less than 0.0014 millimeters). The other method showed an error less than 0.0004 millimeters on average. As for the stress parameter, it was not as accurate as the strain, where the maximum value of the absolute error is large in the end of the beam (-0.6 and 0.6 meters) where the exact solution showed zero value for the stress and the simulations showed a value of -26.0 Pa for RPIM and -11.0 Pa for the EFGM. Although both methods show a good numerical performance, other type of consideration should be taken into account, when choosing one method over another.

The Lagrange multiplier method is one of the most widely used method, however, this method introduces a new unknown function: *the Lagrange multiplier* which is hard to set. The interpolation space for the Lagrange multiplier must be carefully selected in order to obtain an accurate solution, otherwise, the resulting system of equations may become singular if the number of degrees of freedom is too large. On the other hand, the penalty method requires only the choice of one scalar parameter; large values of this parameter must be used in order to impose the boundary conditions in a proper manner. In practice, this leads to ill-conditioned systems of equations, reducing the applicability of the method.

For the case of RPIM, where the shape function follows the Kronecker delta constraints, it was demonstrated that setting the boundary conditions can be applied indifferently for the MFree methods that either fulfill or not the Kronecker delta property.

In the future, we are planning to explore how the other parameters involved in this type of simulations influence the accuracy of the solution, such as, the shape of the support domain, parameters of the radial basis function and the weighed functions.

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