Extending the local radial basis function collocation methods for solving semi-linear partial differential equations

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Abstract

This work addresses local radial basis function (RBF) collocation methods for solving a major class of non-linear boundary value problems, i.e., $Lu = f(x, u)$ being f a non-linear function of u. This class of problems has been largely analyzed in the BEM community.

To our knowledge, few works are reported where the local RBF collocation methods (LRBFCM) based on the generalized Hermite RBF interpolation (double collocation) have been extended successfully to solve semi-linear problems even when extending to more complex nonlinear cases are not reported yet. The studied schemes are based on a strong-form approach of the PDE and an overlapping multi-domain procedure combining with standard iterative schemes. At each sub-domain, a locally meshless approximation solution by a standard or Hermite RBF expansion can be constructed. We studied also the performance respect to the shape parameter of RBF. It is confirmed that the local RBF double collocation can improve greatly the accuracy order. Some *2D* benchmark problems with mixed boundary conditions showing the accuracy, convergence property and implementation issues of LRBFCM are presented.
Keywords: RBF interpolation, double collocation, Domain decomposition methods, semi-linear equation, fully Newton method, Picard iteration.

1 Introduction

The PDE $Lu = f(x, u)$ where x represents the vector of position, u being the field variable and f the only nonlinearity arising from the source term, is encoun-

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tered in heat conduction, chemical rate models, gas dynamics, among other practical applications [1–5]. Its numerical solution in steady-state or unsteady-state with advantaged boundary element methods (BEM) is well established. In the context of dual-reciprocity boundary element method (DRM) [3], it is introduced in turn the normal gradient information at the boundary to improve the needed RBF interpolations (Hermite type) providing more accuracy for permitting additional degree of freedom (DOF) for the same number of interior knots. Extending from this approach in the method of fundamental solution (MFS) is carried out elsewhere [5], improvements of accuracy were also observed when solving aforementioned equations. In unsteady-state solution cases, an efficient formulation that combining DRM and Laplace transforms (LTDRM) can be performed [2]. There a clear advantage of the LTDRM over time-stepping methods was demonstrated through the numerical results, especially if the solution at a particular time is sought. It has been shown that the success relies mainly on the linearization of the nonlinear source term by a first-order Taylor series expansion over u, namely a second-order Picard iteration.

Meshless methods have been proposed and achieved remarkable progress over the past years [6, 7]. They were born with the objective of eliminating part of the inherent difficulties that rely on complex, connected meshes or elements. According to the formulation procedures, they can be mainly classify in global and local weak-forms and global and local strong-forms [8]. For instance, the global element-free Galerkin (EFG) method and the very popular meshless local Petrov-Galerkin (MLPG) method are including under the first group which were developed in 1994 and 1998, respectively [8]. These two methods are widely employed in different complex areas of applications.

On another group of meshless methods, there exists RBF-based methods that have enjoyed tremendous research for solving PDEs. Kansa [9] was the first to use directly globally-supported RBF interpolant, particularly multiquadrics like basis functions, in a point collocation technique to approximate the strong-form of PDEs. Following this idea, Fasshauer [10] suggests to change to generalized Hermite-RBF interpolation. These two techniques are known as unsymmetric and symmetric methods, respectively. The last turns out a collocation matrix that is dense, symmetric and non-singular, whereas Kansa's collocation matrix is dense, non-symmetric and the non-singularity is not guaranteed [11]. This group of meshless methods possesses the following advantages: straight forward process for obtaining discrete equations by directly use the PDE (strong-form), simple implementation, computationally efficient (no numerical integration is required) and truly meshless (by using mainly a meshless interpolation/approximation function). It should be to point out that in [11], the author finds well-suited to solve variable coefficient elliptic and time-dependent PDEs through unsymmetric method. But applying Fasshauer's method to solve a variable coefficient problem finds it very cumbersome. Moreover, he says to be not clear to deal with nonlinear problems using the symmetric method. For a treatment of time-dependent PDEs and one unsteady non-linear heat conduction equation based on the symmetric method together with an implicit time-stepping algorithm looks at [12, 13].

In addition, it has been shown that global RBF collocation methods using some infinitely smooth RBFs are highly accurate and converge exponentially [14]. Even shortcomings are also known as the trade-off principle between the accuracy gained by increasing the c-shape parameter of RBF or the system size and the stability lost due to large matrix condition number created [14], and poor performance accounts for derivative boundary condition [15–17] and non-smooth boundary conditions [18]. To circumvent the ill-conditioning problem and to improve the solution accuracy, several techniques have been explored as matrix preconditioner, multizone methods, variable RBF shape parameter and overlapping and nonoverlapping domain decomposition methods (DDM) [19–22].

A very promising based-LRBFCM have been proposed in [23–27]. They can be seen like a novel implementation of overlapping sub-domain RBF collocation DDM in the limiting case of a very large number of sub-domains. Standard DDM deal with an iterative procedure due to transmission of information for yielding the numerical solution; herein the multi-domain formulation generates a discretized equation for each sub-domain (based on a localized RBF interpolation function) and together with a point collocation technique then arises a global, sparse and well-conditioned collocation matrix as result from an easy assembling process. The major difference between the local RBF methods and the previously presented global ones is the set of unknowns obtained from steady-state governing equations; for the former the unknowns represent the discrete values of the field variable (by defining approximations in term of shape functions) whereas for the latter the unknowns represent the coefficients of a linear combination of basis functions. This is a key step that makes local methods much more flexibility than global ones [25, 26]. For instance, LRBFCM have been more effective than global RBF collocation approaches when solving 2D convection-diffusion problems with moderate-to-high Peclet number [28, 29]. Various strategies have been proposed for determining the number of sub-domain nodes, mostly based on counting the number of them into a specified regular-shaped form of the sub-domains, i.e., circle, rectangles, etc.; or the number of nodes n is fixed and selecting them according to certain criterion, i.e., nearest searching, four quadrant, among other more elaborates [8, 26, 30, 31]. This mild connectivity can be accomplished in a preprocessing stage in the cases that collocation points does not alter its distribution. From here on we will call computational molecules with their star points instead of the so-called sub-domains.

A recent approach was proposed in [32], it aimed to exploit the combination between LRBFCM and the classical control volume (CV) method. There a boundary value problem is solved for every cell and then constructing the cell shape functions from which the evaluation of the flux across the cell faces is obtained. By this way, they were able to improve the performance of the CV method. So far we believe that this approach has been applied successfully to 3D linear convention-diffusion problems for predicting high Péclec number models.

LRBFCM are essentially one truly meshless version that can be applied to large problems reasonably inexpensive and without numerical conditioning issues like 3D problems and Navier-Stokes equations in fluid dynamics, see very recent

papers in [29, 33, 34]. The major goal of this paper is to present new numerical results of LRBFCM for semi-linear problems with further findings compared to few prior implementations [26, 35].

2 PDE model

We consider a PDE model in which the nonlinearities arises from source terms. For simplicity, it has been considered of the form

$$Lu = \Delta u = f(x, u), \quad \text{in } \Omega \tag{1}$$

the boundary conditions are assumed to be of the form

$$u = \overline{u}, \quad \text{on } \Gamma_1 \tag{2}$$

$$q = \frac{\partial u}{\partial \boldsymbol{n}} = \overline{q}, \quad \text{on } \Gamma_2 \tag{3}$$

where u is the unknown field variable, Δ is the Laplacian operator, q is the flux, $\boldsymbol{n}$ being the unit outward normal, $\overline{u}$ and $\overline{q}$ are given functions and $\Gamma = \Gamma_1 \cup \Gamma_2$ is the boundary of the whole problem domain Ω. A fully Newton scheme can be applied straightforward due to the use of the RBF shape functions and discrete values of the field variable.

An alternative numerical treatment is as follow. Let us linearize the nonlinear source term by a first-order Taylor series expansion as

$$f(x, u) =: f_1(x, \widetilde{u}) + f_2(x, \widetilde{u})u \tag{4}$$

where

$$f_1(x, \widetilde{u}) = f(x, \widetilde{u}) - \widetilde{u} \left.\frac{\partial f}{\partial u}\right|_{\widetilde{u}}, \qquad f_2(x, \widetilde{u}) = \left.\frac{\partial f}{\partial u}\right|_{\widetilde{u}} \tag{5}$$

and thus eqn. (1) can be rewritten for a suitable iterative scheme of which arises the Picard iterations

$$L^{\widetilde{u}}u = \Delta u - f_2(x, \widetilde{u})u = f_1(x, \widetilde{u}), \quad \text{in } \Omega \tag{6}$$

where $\widetilde{u}$ is the previously iterated solution and f to be a differentiable function. Note that the discretization of eqn. (6) and its corresponding global system of equations need to be recalculated at each iteration because of new linearized variable coefficient operator depends on the solution iterates.

3 Meshless shape functions and implementations

Let us assume that at each collocation point (node) $x_j \in \theta_h = \{x_j\}_{j=1}^{N}$ is selected (in some way) a subset $S_j \subset \theta_h$, named the computational molecule of x_j such that S_j is the set of surrounding points (centers) of x_j (the star point) which

includes $n << N$ distinct grid-points of which $m \leq n$ could be used in a double collocation way. It assumes that $x_j \in S_j$, and it is the first element. At every molecule S_j, a locally meshless approximate solution $\hat{u}_j$ is sought by a generalized Hermite *RBF interpolation* function augmented with a constant polynomial term [11]:

$$\hat{u}_j(x) = \sum_{i=1}^{n} \lambda_i \phi\left(\|x - \xi_i\|\right) + \sum_{k=1}^{m} \alpha_k \gamma^{\boldsymbol{\xi}} \phi\left(\|x - \xi_k\|\right) + \chi \tag{7}$$

which interpolates both functional values $u(x)$ on all points and derivative information $\gamma u(x)$ at the double collocation points. Note that this interpolant guarantees reproduction of constant functions. If $m = 0$ (the simplest RBF interpolant), it interpolates functional values only, and if $m \neq 0$ then a RBF double collocation is possible to exploit, i.e., in these locations two interpolation conditions are simultaneously satisfied. The latter can be a way to increase the accuracy, without increasing the size of the molecule, whether there is information about the derivatives of the unknown function at some data points. The coefficients of the basis functions have to be determined.

By evaluating the different interpolation conditions into eqn. (7) at the corresponding supporting points n of the molecule for leading to $n + m + 1$ linear equations, that is, n equations by function values, m equations by derivative values and add one standard homogeneous constraint by the polynomial term. The block matrix form of these equations is:

$$\underbrace{\begin{vmatrix} \boldsymbol{\phi}\left(\|x - \xi\|\right) & \gamma^{\xi}\boldsymbol{\phi}\left(\|x - \xi\|\right) & \boldsymbol{e} \\ \gamma\boldsymbol{\phi}\left(\|x - \xi\|\right) & \gamma\gamma^{\xi}\boldsymbol{\phi}\left(\|x - \xi\|\right) & \gamma\boldsymbol{e} \\ \boldsymbol{e}^T & \gamma\boldsymbol{e}^T & 0 \end{vmatrix}}_{A} \begin{vmatrix} \boldsymbol{\lambda} \\ \boldsymbol{\alpha} \\ \chi \end{vmatrix} = \begin{vmatrix} \boldsymbol{u} \\ \boldsymbol{\gamma u} \\ 0 \end{vmatrix} \tag{8}$$

where $\boldsymbol{e}_i = 1$ and the local interpolation matrix A is symmetric, small and nonsingular [26]. As always, the centers ξ and nodes x physically coincide. Also, $\gamma\phi$ is equal to $\gamma^{\xi}\phi$ up to a possible difference in sign [12]. It is worth noting that the interpolation matrix A is a constant matrix for a given star point x_j. As such, it shall change only if the distribution of collocation points or the derivative functional are changed.

Combining eqn. (7) along with the linear system eqn. (8), it leads to that the approximation function can be expressed in term of a linear combination of *meshless shape functions* (called cardinal basis functions in interpolation terminology) with discrete values of the field variable and their derivatives as the coefficients [26]:

$$\hat{u}_j(x) = \sum_{i=1}^{n} u_i \Phi_i(x) + \sum_{k=1}^{m} \gamma u_k \tilde{\Phi}_k(x) \tag{9}$$

like shape functions possess the Kronecker delta property [26] then it is easy to implement the essential (Dirichlet) boundary conditions, e.g., not molecules are

sought at star points belonging to not-derivative boundary. For a linear differential operator $\mathcal{L}$ with variable coefficients, it can be easily discretized by applying to shape functions, i.e.

$$\mathcal{L}\hat{u}_j(x) = \sum_{i=1}^{n} u_i \mathcal{L}\Phi_i(x) + \sum_{k=1}^{m} \gamma u_k \mathcal{L}\tilde{\Phi}_k(x) \tag{10}$$

The derivative functional $\gamma u(x)$ in eqn. (9) can be assumed in several ways for the construction of approximations. Further details on constructing shape functions look at the reference [28]. Herein three options have been proposed

1. When $m = 0$, i.e., it is not assumed a derivative functional as known, so there is not a special treatment for the derivative boundary conditions. This is the simplest formulation that we refer as the local RBF single collocation approach [24].
2. When $m \neq 0$ for molecules that intersect the global derivative boundary since the derivative functional is assumed to come from $\gamma u(x) = \frac{\partial u}{\partial \boldsymbol{n}} = q$. In these m intersecting points within a molecule, their normal derivatives q are included as additional unknowns. At derivative star points, the PDE and the normal derivative boundary condition are satisfied simultaneously with the advantage does not need more meshing work outside the domain; it increases the number of collocation equations needed to close the system. This formulation gives rise to the local RBF double boundary collocation approach [8].
3. When $m \neq 0$ in all molecules since the derivative information is assumed to come from the source term, i.e., $\gamma u(x) = \mathcal{L}u(x) = \mathfrak{f}(x)$. This formulation gives rise to the local RBF PDE collocation approach [26]. In our tests, $m < n$ in interior molecules and $m \leq n$ in molecules with the star point along of the derivative boundary were assumed, reported also in [28]. The former condition rejects explicitly the derivative information at the star point [26].

Applications of whichever above approaches for constructing the approximation functions and the simple point collocation technique, using eqns (1), (2) and (3), lead to a set of nonlinear algebraic equations which can express in the standard valued-vector residual form:

$$\boldsymbol{\varphi}(\boldsymbol{U}) = \boldsymbol{0} \tag{11}$$

where $\boldsymbol{U}$ is the vector of nodal unknowns at all collocation points.

Alternatively, we use eqns (6), (2) and (3) to lead a set of linear algebraic equations at each iteration which can express in the standard matrix-vector notation:

$$\boldsymbol{K}\boldsymbol{U}^{(k)} = \boldsymbol{F} \tag{12}$$

where $\boldsymbol{K}$ is the collocation matrix, $\boldsymbol{U}^{(k)}$ is the vector of unknowns in the kth Picard iteration and the vector $\boldsymbol{F}$ collects the source terms in both the interior and on the boundary. Notice that at each iteration, $\boldsymbol{K}$ and $\boldsymbol{F}$ must be updated. The iteration process is continued until the convergence criteria are satisfied. It is worth noting that the unknown vector $\boldsymbol{U}$ is given term of $(\boldsymbol{u}, \boldsymbol{q})^T$ into eqns (11) and (12) when using the above second option.

4 Numerical evaluations

For eqn. (11) we use a Newton method with line-search, without attempting to optimize, and the Jacobian matrix required by the general-purpose solver is supplied analytically. For deciding the convergence of the solutions by Newton method, tolerances $TolFun = 10^{-7}$ for residual function and $TolX = 10^{-8}$ for incremental correction of the solution vector have been used. For eqn. (12) we use a direct solver in order to invert the linear system and $\left\|U^k - U^{k-1}\right\| / \left\|U^k\right\| < 10^{-4}$ for convergence criterion. In both cases a data structure based on a sparse storage format is used which stores a list of coordinates of non-zero elements. To deal with eqn. (8), it is used an appropriate direct solver in order to invert the small symmetric matrix A. Also the most popular RBF is used, namely $\phi(r) = \sqrt{r^2 + c^2}$ (MQ-multiquadric) along with a constant shape parameter c^2 given by end-user. In our computations, uniformly distributed collocation points and five $n = 5$ and nine nodes $n = 9$ in the molecules have been used. The relative total error norm at the end iteration is taken to measure the accuracy of the numerical results.

For the sake of clarity, we point out the three RBF local methods and their legends that we will use throughout the section. The local single collocation method to be refereed as *meth1*, the local RBF PDE collocation approach to be refereed as *meth2* and the local RBF double boundary collocation method to be refereed as *meth3*. It is worth noting that *meth2* is well suited when the problem has mixed boundary conditions. The other approaches can be well applied to problems with only Dirichlet and also mixed boundary conditions.

4.1 Analytic case

We consider a smooth solution problem in a square domain 1×1 given

$$\begin{aligned} \Delta u &= \exp(-2x)u^3 \quad \text{in } \Omega \\ u &= g \quad \text{on } \Gamma_1 = \{(x,y) \mid y = 0,\ 1,\ 0 \le x \le 1\} \\ \frac{\partial u}{\partial x} &= h \quad \text{on } \Gamma_2 = \{(x,y) \mid x = 0,\ 1,\ 0 < y < 1\} \end{aligned} \tag{13}$$

Exact solution of this problem is

$$u(x,y) = \exp x \tanh \frac{y}{\sqrt{2}} \tag{14}$$

where g and h functions are obtained from the exact solution.

The computations are performed on two uniform point distributions 21×21 ($N = 441$) and 41×41 ($N = 1681$) and different shape parameters ($0.05 < c < 1$). The solution is approximated using meth1 with $n = 5$, meth2 with $n = 9$ and meth3 with $n = 9$. Figure 1 shows the discretization of the domain and the choice of different molecule sizes used in meth1 and meth2.

Figure 2 displays the error norm of the local RBF collocation methods combining with Picard iterations for different c's and two point distributions. In general,

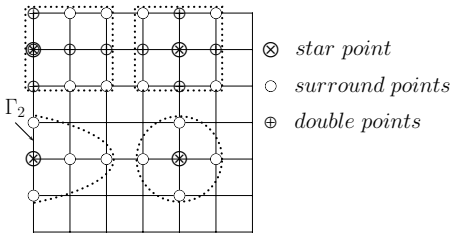

Figure 1: Computational molecules including five and nine supporting points assumed on derivative boundary and internal star points.

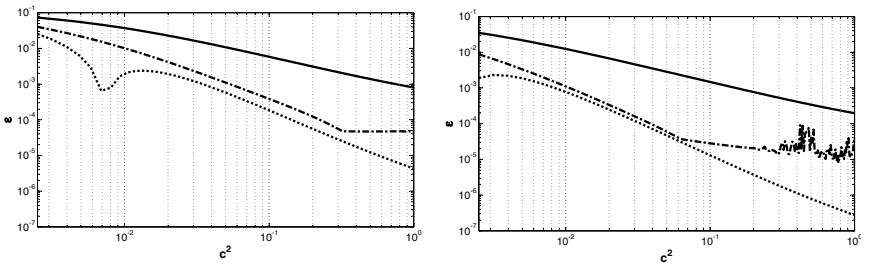

Figure 2: Convergence of the relative error with c^2. Solid line: meth1, dotted line: meth2 and dash-dot line: meth3. On the left uses 21×21 and on the right uses 41×41.

one can see that the error decreases as c increases. Also the error looks to be decreasing as point density increases. Furthermore, we can see also that the accuracy greatly improved using both Hermite collocation approaches (double collocation near and at the derivative boundary and throughout domain), i.e., meth3 and meth2. Accordingly they have the line slope values larger than meth1, i.e., recovering a higher order of accuracy. We observe that beyond to a certain shape parameter presents unavoidable instabilities in the local and/or global systems. To this respect, we felt that *meth1* with a five molecule size is more attractive compared with meth2 and meth3 because less sensitive to c and very much stable and fast computationally. In the present study, at meth1 passing from five to nine molecule size, the computational effort increases more than two times and the error norm does not decrease generally in accordingly (see also [33, 34]). Comparing the meth1 with five molecule size and meth2 with nine molecule size, the former is faster than the latter about 10 times because a less elaborate assembling matrix and less terms in the approximations. Though the latter can be more accurate than the former over 100 times into a wide range of c's. After many tests, on the full range of shape parameter tested, always converged solutions were achieved.

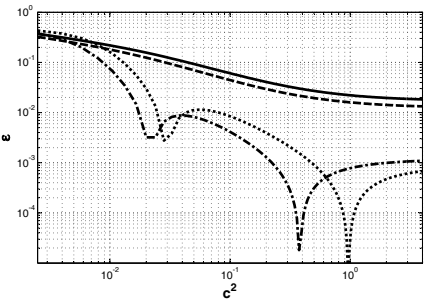

Figure 3: Convergence of the relative error with c^2. Solid line: meth1 and 11×11, dashed line: meth1 and 13×13, dotted line: meth2 and 11×11 and dash-dot line: meth2 and 13×13.

4.2 Kinetic rate problem in a square

Simplified kinetic rate problem in steady-state can be analyzed by means the forced diffusion equation

$$\Delta u = \Psi^2 u^\eta \tag{15}$$

which governs kinetic and diffusional phenomena in a homogeneous medium where Ψ and η are known parameters. Our computations are compared with an exact solution from [4] which is given for $u = 0.4352$ at point $(0, 0)$. There the problem domain is the unit square centered at $(0, 0)$, only Dirichlet boundary condition $u = 1$ is prescribed on whole domain, using $\Psi = 5$ and $\eta = 2$. The computations are performed on two uniform point distributions 11×11 ($N = 121$) and 13×13 ($N = 169$) and different parameters ($0.05 < c < 2$). The other parameters are similar to previous problem.

Figure 3 shows the accuracy of the solution as a function of MQ shape parameter, different point distributions and two local RBF methods combining with Newton method. One can observe also that both methods can achieve an accuracy improvement with higher values of c and denser collocation points. It can be seen that solution error at meth1 decreases very smooth as c increases until to be nearly constant. On the other hand, meth2 (double collocation) is more sensitive to c owing to the error decreases as c increases but now one observes a certain recovery of spectral convergence for a range of c's. Always converged solutions were found with less than five iterations. With this problem, we confirm the applicability of local RBF collocation methods to deal with the simplest nonlinear problems.

5 Conclusions

Here we show that meshless local RBF collocation methods (LRBFCM) are well suited to solve the simplest nonlinear boundary value problems. Particularly we were able to incorporate standard iterative procedures based on fully Newton and

second order Picard methods in all local methods. Though the performance of both procedures was not compared in this work. However, the combination with Newton method can require optimization for reducing the computational cost. In addition, the molecule size can also affect adversely the efficiency due to higher sizes require many computations, e.i., roughly $O(Nn^3)$, see [29]. New details about the performance of the schemes varying the constant shape parameter are shown as such can affect strongly the convergence order and accuracy itself even though it seems dependent on the problems. Furthermore, in the full range of shape parameter tested, always converged solutions were found with few iterations. We are to sure that local RBF methods are quite stables and efficients compared to the counterpart global ones. By the simplicity of these methods, we hope that they can follow up being applied to a wide variety of important applications in the near future.

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