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LOCAL HERMITE-RBF BASED GRID-FREE SCHEME WITH A VARIABLE (OPTIMAL) SHAPE PARAMETER FOR STEADY CONVECTION-DIFFUSION EQUATIONS

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Abstract. In this work, a local algorithm is proposed to optimize the shape parameter of the infinitely smooth Radial Basis Function (RBF) in the local Hermite-RBF (LHRBF) grid free scheme which has been developed to the solve the partial differential equations, in particular, steady Convection Diffusion Equations (CDE), more accurately. The algorithm is based on the re-construction of the forcing term and its (differential) operator value over the centers in the local support domain. A cost function which has similar variation as RMS error function is obtained and the same is minimized to generate a variable shape parameter for each reference center. The LHRBF scheme with the obtained variable (optimal) shape parameter is tested over one and two dimensional steady CDEs to demonstrate its robustness.

Key words. grid-free scheme, radial basis function, convection-diffusion, multiquadric, optimal shape parameter and Hermite-RBF scheme.

1. Introduction

Radial Basis Functions (RBF) are one of the important tools for the interpolation of sparse and scattered data points in multi-dimensions. In the interpolation using RBFs, the function which interpolates the given data is approximated as a linear combination of translates of the radial basis function, which is radially symmetric about its center. The global RBF collocation method for solving partial differential equations was initiated by Kansa [1]. The advantages of the global method are, spectral accuracy, dimensional independence and applicability in irregular geometries. But, the main drawback is the severe ill-conditioning of the global matrix. Wright and Fornberg [2], Chandhini and Sanyasiraju [3], Sanyasiraju and Chandhini [4], have proposed some RBF-based local schemes to overcome the ill-conditioning and tested their schemes over Poisson, convection-diffusion and incompressible flow equations. These discretization schemes were developed using collocation over some local support domains, therefore, the resulting global matrices were sparse and better conditioned but lost their spectral accuracy.

Based on the Hermite-Brikhoff interpolation [5], a higher order local RBF scheme, over scattered nodes, is proposed by Wright and Fornberg [2] which is the generalization of the method introduced by Collatz [6] and Lele [7], for scattered nodes. In this method, the (differential) operator is approximated as a linear combination of the function values and also its operator values over the nodes in a local support domain. Wright and Fornberg [2] tested their scheme by generating numerical solutions for the linear and nonlinear elliptic type equations. In these numerical experiments, the shape parameter of the Multi-Quadric (MQ) RBF is prefixed randomely.

There exists many types of RBFs in the literature, like Multi-Quadric, Gaussian, Inverse Multi-Quadric and Thin Plate Splines. Among them, Multi-Quadric (MQ),

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LHRBF GRID-FREE SCHEME WITH A VARIABLE (OPTIMAL) SHAPE PARAMETER 383

 $\phi(r) = \sqrt{(1 + (\varepsilon r)^2)}$, where $r = ||\underline{x}||_2$, $\underline{x} \in \mathbb{R}^d$, d- is the dimension of the problem, ε is the shape parameter, is more popular due to its better approximation property [8]. However, for MQ the scaling (shape) parameter plays a significant role in obtaining accurate solutions. In most of the existing literature, researchers have chosen the shape parameter either by trail and error or by some ad hoc means. This strategy may not give accurate solutions when the problems having non-smooth solutions like the Convection-Diffusion Equations (CDE) are solved. The steady form of CDE is given by

- (1) $\mathscr{L}u(\underline{x}) = f(\underline{x}), \, \forall \, \underline{x} \in \Omega \subset \mathbb{R}^d,$
- (2) $\mathscr{B}u(x) = g(x), \forall x \in \partial\Omega \subset \mathbb{R}^d,$

where $\mathscr{L} = \overline{b} \cdot \nabla - a\Delta$, $\overline{b} \cdot \nabla = b_j \partial / \partial x_j$, $\Delta = \partial^2 / \partial x_j x_j$, $\overline{b}(\underline{x})$, is the convection coefficient, a is the diffusion coefficient, $\mathscr{B} = \alpha + \beta \partial / \partial x_j$ is the boundary operator; depending on the values of α and β , it can be a Dirichlet, Neumann or a mixed operator, Ω is a bounded domain, $\partial \Omega$ is the boundary of Ω .

There are some attempts in the literature [1, 8, 9] to optimize the shape parameter of the infinitely smooth RBFs, when they are used in the interpolation problems. Rippa [10] proposed a "leave-one-out" cross-validation (LOOCV) algorithm for finding an optimum value of the shape parameter for the RBF interpolation. Fasshauer [11] and Roque [12] extended the LOOCV algorithm for finding the optimal shape parameter for the global collocation in solving the partial differential equations. Cheng et al. [13] have shown that, for the global RBF methods, the optimal shape parameter lies in the region where the global matrix is highly ill-conditioned. To combat this problem, Sanyasiraju and Satyanarayana [14] have developed a local optimization algorithm to optimize the shape parameter for LRBF schemes. This local algorithm is developed based on the reconstruction of the forcing term of the CDE over the local supporting domain of any reference point \underline{x}_i .

In the present work, the local optimization algorithm [14], which is developed for the LRBF scheme, is extended for the LHRBF scheme. This local algorithm is developed based on the re-construction of the forcing term and its (differential) operator value over the local support domain of the reference point \underline{x}_i . The local cost function of the proposed algorithm is defined in terms of the residual errors. The spatially variable (optimal) shape parameter is obtained by minimizing the local cost function at each center of the computational domain. The LHRBF scheme with the variable (optimal) shape parameter is validated using one and two dimensional steady CDEs and demonstrated its performance.

Rest of the paper is organized as follows. In Section 2, the development of the Local Hermite-RBF grid free scheme is described. In Section 3, the derivation of the proposed local optimization algorithm is presented. Implementation and the validation of the local optimization algorithm, by applying it to solve several CDEs are presented in the Section 4. Finally, some concluding remarks are made in the last section.

2. Local Hermite-RBF grid-free scheme

In the local RBF grid-free schemes [3, 4], at any reference center, the differential operator is approximated as a linear combination of the function values on the local support region of the reference point. In order to improve the accuracy of the local RBF grid-free scheme, we consider not only the function values but also its operator values on the centers, without increasing the size of the local supporting region. The schematic diagrams of the 3 and 9 point stencils for the discretization