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A RBF Based Local Gridfree Scheme for Unsteady Convection-Diffusion Problems

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Abstract

In this work a Radial Basis Function (RBF) based local gridfree scheme has been presented for unsteady convection diffusion equations. Numerical studies have been made using multiquadric (MQ) radial function. Euler and a three stage Runge-Kutta schemes have been used for temporal discretization. The developed scheme is compared with the corresponding finite difference (FD) counterpart and found that the solutions obtained using the former are more superior. As expected, for a fixed time step and for large nodal densities, though the Runge-Kutta scheme is able to maintain the higher order of accuracy over the Euler method, the temporal discretization is independent of the improvement in the solution, which in the developed scheme, has been achieved by optimizing the shape parameter of the RBF.

Keywords: radial basis function; multiquadric: local; unsteady; convection-diffusion.

1. Introduction

The convection-diffusion process plays a very significant role in fluid flow and heat transfer problems. This process is peculiar in the sense that it is a combination of two dissimilar phenomena, convection and diffusion. It can also be viewed as a simplified model problem for the governing equations of the fluid flow, i.e, Navier-Stokes equations. This makes the numerical prediction of the solution of the convection-diffusion equation very important in computational fluid dynamics. The unsteady convection-diffusion equation is given by

$$\frac{\partial u(\bar{x},t)}{\partial t}+\bar{a}.\nabla u(\bar{x},t)-D\nabla^2 u(\bar{x},t)=f(\bar{x},t),\ \bar{x}\in\Omega\subseteq\mathbb{R}^d, t>0 \tag{1}$$

with general initial and boundary conditions.

$$\alpha_1 u(\bar{x},t)+\alpha_2\nabla u(\bar{x},t)=g(\bar{x},t), \bar{x}\in\Omega, t>0 \tag{2}$$

$$u(\bar{x},t)=u_0(\bar{x}), t=0, \bar{x}\in\Omega\bigcup\partial\Omega \tag{3}$$

where $u(\bar{x},t)$ is the unknown to be computed, d is the dimension of the problem, Ω is a bounded domain in $\mathbb{R}^d$, $\partial\Omega$ is the boundary of Ω, D is the diffusion coefficient, $\bar{a}=(a_1,\ldots,a_d)$ is the

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convection coefficient, $\nabla = e_j \dfrac{\partial}{\partial x_{e_j}}$ is gradient operator, $\nabla^2 = \dfrac{\partial^2}{\partial x_{e_j} \partial x_{e_j}}$, α_1 and α_2 are known constants, and $f(\bar{x},t)$, $g(\bar{x},t)$ and $u_0(\bar{x})$ are known functions.

The numerical computation of the solution of the convection-diffusion problem, described in equations (1)-(3) becomes very challenging when the convective process is dominant over diffusion. That is, the dimensionless parameter that measures the relative strength of the diffusion (D) over convection is very small. In such situations numerical approximations get contaminated due to the spurious oscillations and numerical diffusion. In the present work, the local radial basis function (RBF) based scheme [1, 2] has been used to solve transient convection-diffusion equations.

Kansa [3] initiated the use of RBFs in the global collocation methods for solving partial differential equations (PDEs). Following this, Fasshauer [4] proposed another collocation method based on Hermite-RBF interpolation. Due to the global nature of these methods, the linear algebraic systems ultimately obtained in these schemes are highly dense and ill-conditioned. To circumvent this, recently, an RBF based local method has been proposed by Wright et al [2]. Chandhini and Sanyasiraju [1] has extended the RBF local scheme to linear and non-linear coupled steady convection-diffusion equations in one and two dimensions and demonstrated that by varying the shape parameter of the radial basis functions the solutions of steady convection-diffusion equations can be made non-oscillatory.

The temporal discretisation has been tested with Euler and also with a three stage Runge-Kutta scheme. The main purpose of this work is to highlight the advantage of localness of the developed gridfree scheme and also to demonstrate how an optimum shape perameter of the RBF generates more accurate solutions than its finite difference counterpart for time dependent convection diffusion equations. The developed scheme has been validated using some one and two dimensional problems with sharp gradients. Solutions are obtained for the diffusion parameter as small as 0.01. Multiquadric (MQ) (17) has been used in all the reported numerical experiments due to its excellent performance over the other RBFs. It has been proved by Driscoll and Fornberg [5] that, for infinitely smooth RBFs like MQ, as the shape parameter $\varepsilon \to 0$ in one dimension, these interpolants converge to Lagrange interpolant. Hence, as $\varepsilon \to 0$, the classical FD solutions can be reproduced from the present local RBF scheme. However, to produce non-oscillatory solutions the optimum non-zero ε has been exploited in all the computations.

2. RBF approximation of unsteady convection-diffusion equation

2.1. RBF approximation of space operator

A function $\Phi : \mathbb{R}^d \to \mathbb{R}$ is called *radial* provided there exists a univariate function $\phi : [0,\infty) \to \mathbb{R}$ such that $\Phi(\bar{x}) = \phi(r)$, where $r = \| \bar{x} \|$ and $\| . \|$ is some norm on $\mathbb{R}^d$. Radial Basis Functions (RBFs) are well-known for approximating multivariate functions, especially from a sparse and scattered set of data. Let L be the stationary part of the convection-diffusion operator given by $\bar{a}.\nabla - D\nabla^2$ and $\bar{x}_i$ be any point in the domain Ω. Consider a set S_i, consisting of n_i neighboring nodes of $\bar{x}_i$, given by $S_i = \{\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_{n_i}\}$. To approximate $Lu(\bar{x}_i)$, let it be represented as a linear combination of u at the points of S_i, given by

$$Lu(\bar{x}_i) = \sum_{j=1}^{n_i} c_j u(\bar{x}_j) \tag{4}$$

Then, the computation of the weights c_j gives the required approximation to $Lu(\bar{x}_i)$. Applying the operator L to the Lagrange representation of the approximate solution

$$s(\bar{x}) = \sum_{j=1}^{n_i} \psi_j(\bar{x}) u(\bar{x}_j) \tag{5}$$

where $s(\bar{x})$ is the interpolation function of u at $\bar{x}$ and $\psi_j(\bar{x})$'s are the Lagrange functions satisfy the cardinal conditions,

$$\psi_j(\bar{x}_k) = \delta_{jk},\ j,k = 1,2,\ldots,n \tag{6}$$

gives,

$$Lu(\bar{x}_i) \approx Ls(\bar{x}_i) = \sum_{j=1}^{n_i} L\psi_j(\bar{x}_i) u(\bar{x}_j) \tag{7}$$

From equations (4) and (7), c_j 's can be obtained as,

$$c_j = L\psi_j(\bar{x}_i) \tag{8}$$

Approximation to each ψ_j, $j = 1,2,\ldots,n_i$ in terms of RBFs can be obtained by expressing them as,

$$\psi_j(\bar{x}) \approx \sum_{k=1}^{n_i} \lambda_{jk} \phi(\| \bar{x} - \bar{x}_k \|) + \sum_{k=1}^{l} \gamma_{jk} p_k(\bar{x}),\ \ j = 1,2,\ldots,n_i \tag{9}$$

where $\phi(\| \, . \, \|)$ is some radial function, $\{p_j(\bar{x})\}_{j=1}^{l}$ is a basis for Π_m^d (space of all d-variate polynomials with degree $\le m$) and l is the dimension of Π_m^d. The weights λ_{jk} and γ_{jk} can be obtained by imposing the cardinal conditions (6) and orthogonality conditions

$$\sum_{j=1}^{n_i} \lambda_j p_k(\bar{x}_j) = 0,\ k = 1,\ldots,l \tag{10}$$

on the approximation (9). Combining (9) and (10) together as a system gives

$$\begin{pmatrix} \Xi & p \\ p^T & 0 \end{pmatrix} \begin{pmatrix} \bar{\lambda} \\ \bar{\gamma} \end{pmatrix} = \begin{pmatrix} e_j \\ 0 \end{pmatrix} \tag{11}$$

where $\Xi_{ij} = \phi(\| \bar{x}_i - \bar{x}_j \|),\ j = 1,\ldots,n_i$, $p_{ij} = p_j(\bar{x}_i),\ j = 1,\ldots,l$ and $i = 1,\ldots,n_i$ and e_j is a vector whose jth element is one and rest are zeros. Also, for the further reference call the coefficient matrix in (11) as A. Solving (11) for $\bar{\lambda}$ and $\bar{\gamma}$ using Crammer's rule gives $\lambda_{jk} = \frac{|A_k|}{|A|}$, where $|A_k|$ is the determinant of the matrix A after replacing the k^{th} column with e_j. In this computation value of k between 1 and n_i gives $\bar{\lambda}$ and between n_i+1 to n_i+l gives $\bar{\gamma}$. Using the values of $\bar{\lambda}$ and $\bar{\gamma}$ in (9) gives (for $j = 1,\ldots,n_i$)

$$\psi_j(\bar{x}) \approx \frac{1}{|A|} \left[\sum_{k=1}^{n_i} |A_k| \, \phi(\| \bar{x} - \bar{x}_k \|) + \sum_{k=1}^{l} |A_{n_i+k}| \, p_k(\bar{x}) \right]$$

$$\psi_j(\bar{x}) \approx \frac{1}{|A|} \left[\sum_{k=1}^{n_i} (\textbf{\textit{Cofactor of}}\ \Xi_{jk}) \phi(\| \bar{x} - \bar{x}_k \|) + \sum_{k=1}^{l} (\textbf{\textit{Cofactor of}}\ \boldsymbol{p}_{jk}) \, p_k(\bar{x}) \right]$$

$$\psi_j(\bar{x}) \approx \frac{|A_j(\bar{x})|}{|A|} \tag{12}$$

where $|A_j(\bar{x})|$ is the determinant of the matrix A after replacing its j^{th} row with the vector $B(\bar{x})$ given by

$$B(\bar{x}) = \left[\phi(\|\bar{x}-\bar{x}_1\|, \phi(\|\bar{x}-\bar{x}_2\|, \ldots\ldots, \phi(\|\bar{x}-\bar{x}_{n_i}\| \,\Big|\, p_1(\bar{x}), p_2(\bar{x}), \ldots\ldots, p_l(\bar{x})\right]^T \tag{13}$$

Using the definition of j (12) in (8) and making use of the symmetry of the interpolation matrix one can write

$$L(\psi_j(\bar{x})) \approx \frac{L(|A_j(\bar{x})|)}{|A|} \tag{14}$$

Therefore from (8) and (14)

$$c_j \approx \left.\frac{L(|A_j(\bar{x})|)}{|A|}\right|_{\bar{x}_i}, \quad j = 1, \ldots, n_i \tag{15}$$

Then, applying the Crammer's rule in reverse manner leads to,

$$\begin{pmatrix} \Xi & p \\ p^T & 0 \end{pmatrix} \begin{pmatrix} \bar{c} \\ \bar{\mu} \end{pmatrix} = \left(L[B(\bar{x}_i)]\right) \tag{16}$$

where $\bar{\mu}$, a dummy vector corresponding to the vector $\bar{\gamma}$ in (9).

It is clear from (15) that though it is dense, the size of (16) is only n_i, which is very much smaller than the size n of the global RBF collocation system. This makes the system more stable for wide range of ε. Further, in (16), only the right hand side depends on the operator L for which the weights have to be computed. This optimizes the computational time when weights are to be computed for many operators with same distribution of nodes, as in the case of non-linear equations and even more useful for time dependent problems, wherein the weights have to be computed for every time level. This has been exploited in the present computations while applying the scheme at different time levels.

Franke [6], has made a comprehensive comparison of about seven groups comprising of about 30 interpolation methods on six different test functions and found that performance of multiquadric (MQ) is the most impressive and consistently performed better in terms of accuracy. Therefore, the multiquadric function, defined by

$$\phi(r) = \sqrt{1 + r^2} \tag{17}$$

where $\varepsilon > 0$, has been used in all the computations presented in this work.

2.2. Temporal approximation

The temporal approximation of the unsteady convection-diffusion equation

$$\frac{\partial u(\bar{x},t)}{\partial t} = \underbrace{-\bar{a}.\nabla u(\bar{x},t) + D\nabla^2 u(\bar{x},t) + f(\bar{x},t)}_{L} \tag{18}$$

is achieved by Euler and a 3-Stage Runge-Kutta (RK) methods.

2.2.1 *Euler method:*

$$\frac{u^{(n+1)} - u^{(n)}}{\Delta t} = L[u^{(n)}] \;\Rightarrow\; u^{(n+1)} + \Delta t\, L[u^{(n)}] \tag{19}$$

2.2.2 *3-Stage Runge-Kutta method:*

$$\begin{aligned} &\text{Stage 1: } u^{(n+1/3)} = u^{(n)} + \Delta t\, \bar{L}[u^{(n)}] \\ &\text{Stage 2: } u^{(n+2/3)} = \frac{1}{4}\left\{3u^{(n)} + u^{(n+1/3)} + \Delta t\, \bar{L}[u^{(n+1/3)}]\right\} \\ &\text{Stage 3: } u^{(n+1)} = \frac{1}{3}\left\{u^{(n)} + 2u^{(n+2/3)} + 2\Delta t\, \bar{L}[u^{(n+2/3)}]\right\} \end{aligned} \tag{20}$$

where Δt is the time step and $\bar{L}[u]$ is the local RBF space discretization, obtained using the procedure described from (4) to (17).

3. Numerical Illustrations

3.1 One dimensional problem

Consider the one dimensional (1D) example problem

$$\frac{\partial u}{\partial t} + a_1 u_x - D u_{xx} = f(x,t),\; 0 < x < 2,\; t > 0 \tag{21}$$

with analytical solution

$$u(x,t) = \frac{1}{4t+1} e^{-\frac{(x-a_1 t-0.5)^2}{D(4t+1)}},\; 0 \le x \le 2, t \ge 0 \tag{22}$$

Initial and boundary conditions and the source term f have been taken from the given analytical solution (22). For the Example (21), results are obtained for the parameters a_1 = 0.8 and D = 0.01. The number of nodal points has been taken as 21, 41 and 81. Though the different nodal distributions considered are of uniformly spaced, the gridfree nature of the method has been exploited by increasing the number of supporting nodes (n_i). That is, for one dimensional problem, the number of supporting nodes n_i has been varied between 3 and 5. The flexibility in the number of supporting nodes comes with no extra effort for RBF scheme, while in FD the scheme itself has to be re-formulated.

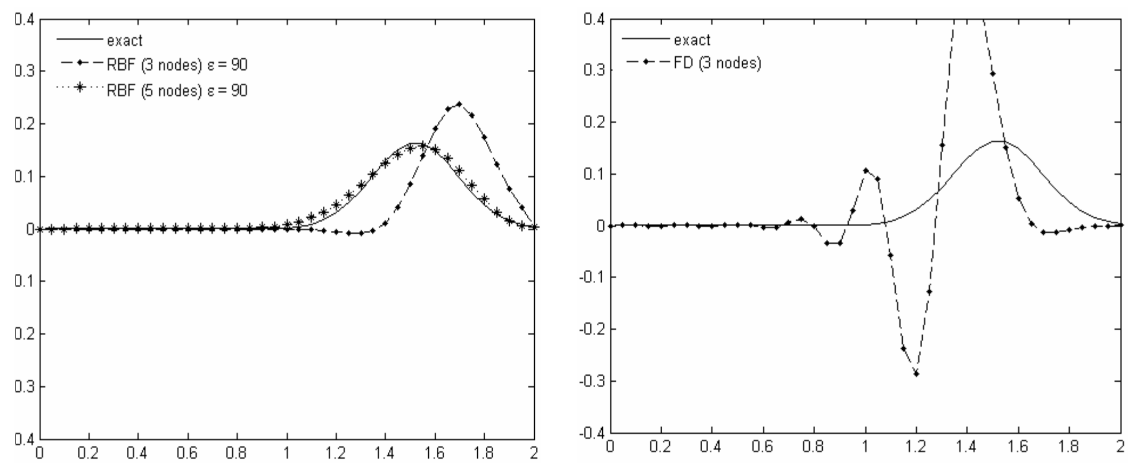
TABLE 1: COMPARISON OF ERROR (err_∞) AND RATE OF CONVERGENCE FOR 1D EXAMPLE WITH DIFFERENT SUPPORT DOMAINS

No. of	Euler based RBF			3-stage R-K based RBF		
nodes	21	41	81	21	41	81
n_i = 3	3.23(-02)	9.70(-03)	2.50(-03)	3.12(-02)	8.90(-03)	2.00(-03)
rate	--	1.7	2.0	--	1.8	2.2
n_i = 5	2.60(-02)	8.00(-04)	7.00(-04)	2.57(-02)	5.00(-04)	1.65(-05)
rate	--	5.0	0.2	--	5.7	4.92

Errors (based on ∞-norm) and the rates of convergence are presented in the Table 1. In these tables, the results obtained using Euler and 3-stage R-K schemes have been compared for different grid densities. In all these computations, the convergence rate has been computed using

$$rate = \frac{\log(E^h / E^{h/2})}{\log(2)} \tag{23}$$

where E^h and $E^{h/2}$ are the errors with the grid sizes h and $h/2$, respectively. A relatively larger time step (Δt) 0.0365 has been fixed in all the computations. It is clear from these



(a) (b)

Figure 1. Comparison of the solutions for 1D problem at t = 1.25, (a) RBF solutions with n_i = 3, 5 (b) FD solution with n_i = 3

comparisons that the number of nodes in the supporting domain influences the rate of convergence. For example, with n_i = 3, the RBF scheme approximately gave 2nd order rate of convergence, but has been improved to 4 once n_i has been increased to 5. The improvement in the convergence rate is visible both in Euler and RK based schemes, however, when the number of nodes is increased from 41 to 81, Euler scheme failed to maintain the higher rate of convergence indicating the need for reduction in the time step. On the other hand there is no such problem with the Runge-Kutta based RBF scheme and it is able to maintain the 4th order rate of convergence. Figures 1(a) and 1(b) present the solutions obtained using RBF and FD schemes, respectively. The smooth RBF based solutions are obtained by varying the shape parameter (reported in Figures 1(a)). It is again evident from this comparison that when the finite difference solution is highly oscillatory, the RBF solution is non-oscillatory though it is slightly erroneous. Further, the RBF solution becomes very accurate once the number of nodes in the local support domain has been increased to five.

3.2 . Two dimensional problem

Consider the one dimensional (1D) example problem

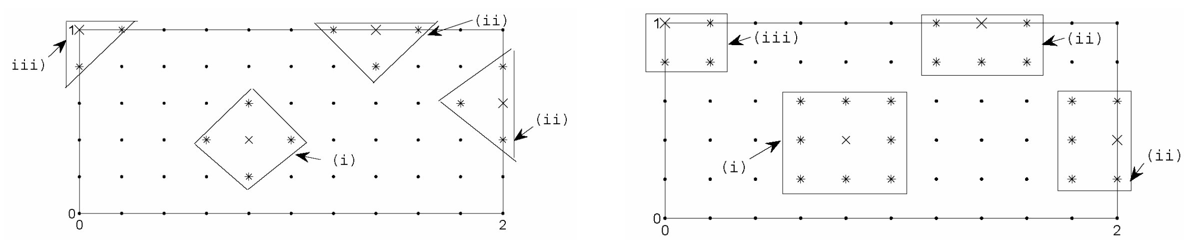
$$\frac{\partial u}{\partial t}+(a_1,a_2).(u_x,u_y)-D(u_{xx}+u_{yy})=f(x,y,t),\ 0<x,y<2,\ t>0 \tag{24}$$

with analytical solution

$$u(x,y,t)=\frac{1}{4t+1}e^{\frac{-(x-a_1t-0.5)^2}{D(4t+1)}-\frac{(y-a_2t-0.5)^2}{D(4t+1)}},\ 0\le x,y\le 2 \tag{25}$$

TABLE 2: COMPARISON OF ERROR (err_∞) AND RATE OF CONVERGENCE FOR 2D EXAMPLE WITH DIFFERENT SUPPORT DOMAINS

No. of nodes	Euler based RBF			3-stage R-K based RBF		
	21x21	41x41	81x81	21x21	41x41	81x81
$n_i = 5$	1.20(-02)	3.71(-03)	9.81(-04)	1.19(-02)	3.68(-03)	9.45(-04)
rate	--	1.7	1.9	--	1.7	2.0
$n_i = 9$	6.61(-03)	3.94(-04)	3.74(-04)	6.54(-03)	1.85(-04)	1.25(-05)
rate	--	4.1	0.07	--	4.1	3.9



(a) (b)

Figure 2. A typical 2D domain discretised with (a) 5-node, (b) 9-node support domains (i) internal, (ii) boundary and (iii) corner nodes

Initial and boundary conditions and the forcing function f have been taken from the given analytical solution (25). For the 2D problem (24) the parameters are fixed as $a_1 = a_2 = 0.8$ and $D = 0.01$ and the Table 2 gives the corresponding err_∞ and order of convergence. For this example again to improve the accuracy, the number of nodes in the support domain has been increased as shown in the Figure 2. The corresponding surface plots are presented in Figure 3 which makes a comparison between RBF and FD solutions. It is clear from this comparison that when the finite difference method over predicts the peak of the solution the RBF solution with nine supporting nodes is very accurate. It is also evident from the Table 2 and Figure 3, that the behaviour of the solution is similar to the corresponding one dimensional example.

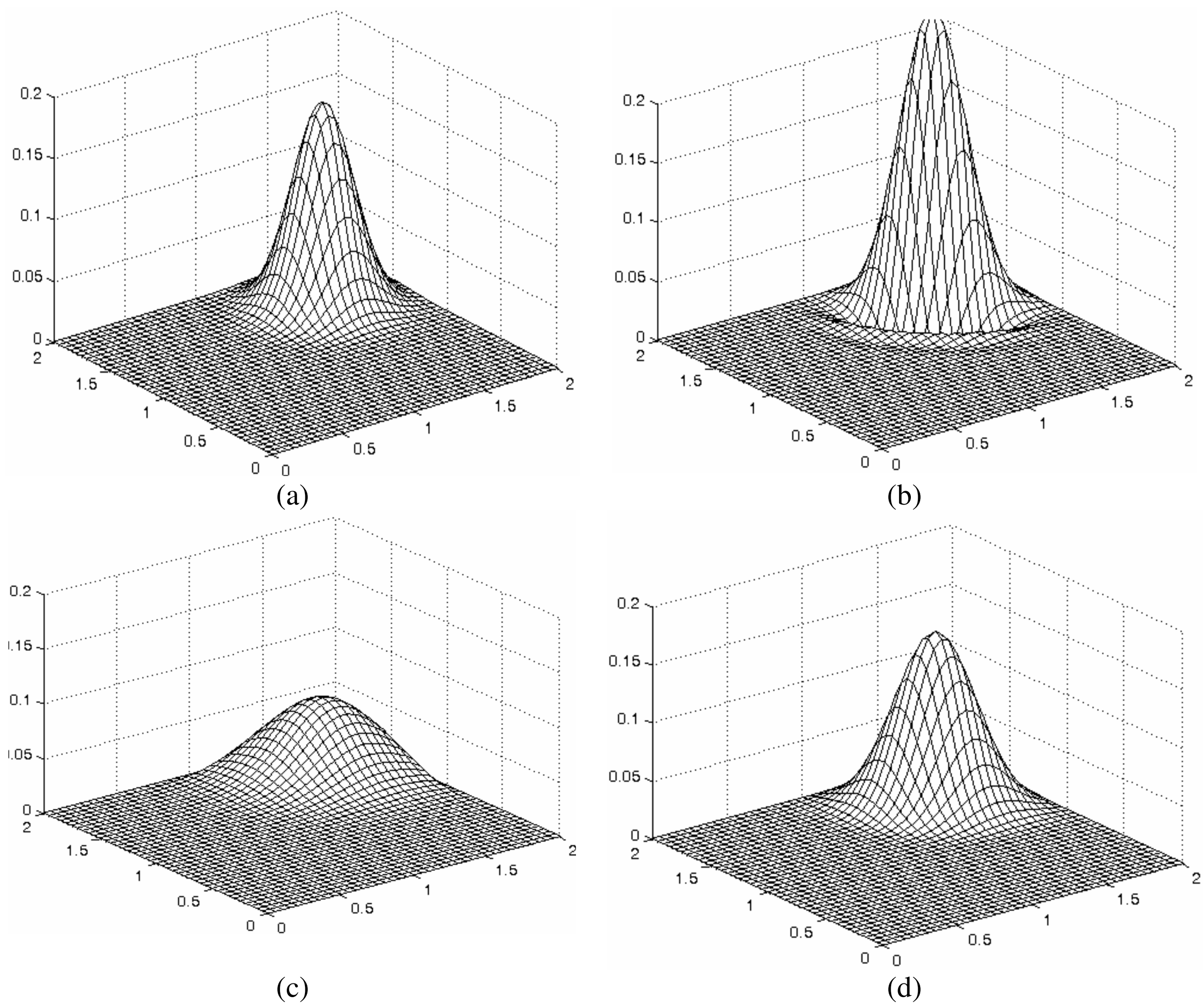


Figure 3. Comparison of the solutions for 2D problem at t = 1.25, (a) Exact Solution (b) FD solution - ni = 5, (c) RBF solution - ni = 5 (ε = 80) & (d) RBF solution - ni = 9 (ε = 80)

4. Conclusion

In the present article, a radial basis function based local numerical scheme for unsteady convection-diffusion equations has been experimented. The method of lines has been used to decouple the time and space operators. Explicit Euler and a computationally economical Runge Kutta method have been used to discretise the time derivative. The complete derivation of the gridfree local scheme for the space discretization of a general time dependent differential operator has been included. Numerical studies for both one and two dimensional convection-diffusion equations have been carried out. To compare the method with the standard finite difference scheme, uniform distribution of nodal points has been chosen, though the developed scheme has a natural mechanism to carry out computations over scattered nodal distributions. The convection-diffusion parameter, D, has been fixed as 0.01. Even for such small values of D, for which FD solutions are oscillatory, the developed local RBF scheme has provided accurate results. The high accuracy is achieved by tuning the shape parameter ε. That is, for convection dominated problems, oscillations are suppressed by increasing the value of ε and also by increasing the number nodes in the support domain. It is known that for RBFs having the parameter ε, there will be a trade-off between the accuracy and the stability with respect to the parameter. This is also been observed in the current analysis that for small values of ε it is seen that the rate of convergence gradually decreased with the increase in the grid density. However in such cases the accuracy of the scheme has been improved by increasing the number of nodes in the support domain, which comes with no extra effort in the developed scheme unlike the corresponding finite difference approximations. The optimum value of the parameter ε has been obtained by trial and error base and its value for each problem has been reported. Further the improvement of the solutions obtained using the developed local scheme is independent of the temporal approximation as it is shown that for both Rugne-Kutta and Euler time derivative approximations the developed scheme gave better solutions than the conventional finite difference method. To summarize, the localness of the developed gridfree scheme and optimization of the shape parameter of the RBF can be exploited to generate more accurate solutions for the time dependent convection diffusion equations over finite difference and also over global grid free RBF schemes which are computationally expensive.

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