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An Upwind Scheme to Solve Unsteady Convection-Diffusion Equations using Radial Basis Function based Local Hermitian Interpolation Method with PDE Centres

K. Monysekar*, Y.V.S.S. Sanyasiraju

Department of Mathematics, Indian Institute of Technology Madras, Chennai - 600036, India

Abstract

Spurious oscillations occur in the numerical results of convective dominated problems with discontinuities when central interpolation schemes are used. Upwind interpolation is necessary to overcome these oscillations. In this work, an upwind scheme is proposed to solve the unsteady convection-diffusion equation using Radial Basis Function (RBF) based Local Hermitian Interpolation (LHI) with PDE centres. It is a meshless numerical method based on the interpolation of overlapping RBF systems and also satisfy the governing partial differential equations at certain specified locations. Local hermite interpolation gives symmetric non-singular interpolation matrix which can be inverted easily to solve the system of equations. The scheme is implemented to unsteady benchmark problems and validated against the corresponding analytical solutions. Comparisons with the benchmark solutions show that the proposed upwind scheme is stable and produces significantly accurate results especially for convection dominated problems.

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Keywords: Upwind, Convection; Diffusion; Radial Basis Function; Hermitian; Interpolation.

1. Introduction

In Gridfree schemes solution is approximated on a set of solution centres scattered in the solution domain with no specified connectivity. Gridfree schemes based on Radial Basis Functions (RBFs)have high order of convergence.

Kansa [1] used RBF interpolation in the global way for solving PDEs followed by Fasshauer [2] and Wu [3] with Hermite-RBF interpolation. The collocation matrix obtained by Fasshauer is symmetric and non-singular, while the matrix obtained by Kansa is non-symmetric and need not be non-singular. These methods produce ill-conditioned matrix system when the size of the data set increases. Local Hermitian Interpolation (LHI) is one such technique to get away with this. In this method, the discretization of the derivatives at any particular point is obtained by the interpolation of RBF using a small set of neighbouring points. Since the individual RBF systems never grow large, such method can be applied to large data sets without numerical ill conditioning.

* Corresponding author. Tel.: +0-000-000-0000 ; fax: +0-000-000-0000.
E-mail address: k.monys@gmail.com

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In the present work, an upwind scheme is proposed based on the interpolation technique adopted by Henry Power et al [4] to solve unsteady convection-diffusion problems. The speciality of the method is inclusion of the boundary operator within the basis functions allowing a natural description of the boundary conditions and inclusion of the PDE operator to the basis functions satisfy the governing PDE at certain prefixed locations.

The organization of the paper is as follows: the Local Hermitian Interpolation (LHI) technique using RBFs and the development of the grid free scheme to solve Initial Boundary Value Problems (IBVPs) is presented in Section 2. The proposed Upwind scheme is explained in Section 3. In Section 4, the developed scheme has been validated for some of the unsteady benchmark problems and compared the results with the exact values.

2. RBF based LHI with PDE centres

Consider a general Initial Boundary Value Problem (IBVP)

$$\frac{\partial u(x,t)}{\partial t} = L[u(x,t)] + S'(x) \qquad in \;\; \Omega$$

$$u(x,0) = f(x)$$

$$B[u(x,t)] = g(x,t) \qquad on \;\; \partial\Omega$$

where $\bar{L}[\;\;]$ and B[ ] are some linear partial differential operators. Applying finite difference approximation in time derivative, the equation becomes

$$\frac{u^n - u^{n-1}}{\Delta t} = \theta L[u^n] + (1-\theta)L[u^{n-1}] + S'(x)$$

The modified equation is obtained as follows by rearranging the terms and simplifying the equation

$$\bar{L}[u^n] = \hat{L}[u^{n-1}] + \Delta t S'(x)$$

where

$$\bar{L} = 1 - \theta\Delta t L, \qquad \hat{L} = 1 + (1-\theta)\Delta t L$$

The original IBVP is now reduced, at each time step, to a steady BVP with the right hand side term given in terms of the solution of the problem at the previous time step. Aim is to solve the BVP.

The RBF $\Psi(\|x-\xi_j\|)$ which is chosen in these computations as the multi-quadric function which depends on the distances between the set of functional centers $\{\xi_j \in \mathbb{R}^n;\, j = 1, 2, ..., N\}$ and maintains symmetry around these points. In order to obtain a non-singular interpolation matrix, the multi-quadric functions of order m require the addition of a polynomial term of order m-1 and an additional homogeneous constraint.

The solution space Ω is covered by two sets of data, locations at which the solution value and the PDE operator are enforced within the interpolation function. Data centres are also placed on all the boundary surfaces $\partial\Omega$. Each solution data centre has associated with it a local system comprised of other solution centres and also PDE and boundary centres. The solution is approximated using a series of hermitian interpolations on each of the local systems using the functional values for solution centres, the source term value for PDE centres and the boundary operator values at boundary centres. In this way, at each local system the field variable $u(x)$ is approximated by

$$u^{(k)}(x) = \sum_{j=1}^{NS} \alpha_j^{(k)} \Psi(\|x-\xi_j\|) + \sum_{j=NS+1}^{NS+NB} \alpha_j^{(k)} B_\xi[\Psi(\|x-\xi_j\|)] + \sum_{j=NS+NB+1}^{NS+NB+NPDE} \alpha_j^{(k)} \bar{L}_\xi[\Psi(\|x-\xi_j\|)]$$

$$+ \sum_{j=1}^{NP} \alpha_{j+N} P_{m-1}^j(x)$$

where

$$k - \text{Local system Index}, \quad NS - \text{No of Solution Centres}, \quad NB - \text{No of boundary centres}$$

$$NPDE - \text{No of PDE centres}, \quad NP - \text{No of terms in the polynomial}$$

This interpolation leads to a symmetric linear systems $A^{(k)}\alpha^{(k)} = d^{(k)}$, for each local domain, which can be solved independently to interpolate the solution over Ω where

$$A^{(k)} = \begin{bmatrix} \Psi_{ij} & B_\xi[\Psi_{ij}] & \bar{L}_\xi[\Psi_{ij}] & P_{m-1} \\ B_x[\Psi_{ij}] & B_x B_\xi[\Psi_{ij}] & B_x\bar{L}_\xi[\Psi_{ij}] & B_x[P_{m-1}] \\ \bar{L}_x[\Psi_{ij}] & \bar{L}_x B_\xi[\Psi_{ij}] & \bar{L}_x\bar{L}_\xi[\Psi_{ij}] & \bar{L}_x[P_{m-1}] \\ P_{m-1}^T & B_\xi[P_{m-1}]^T & \bar{L}_\xi[P_{m-1}]^T & 0 \end{bmatrix} \text{and} \quad d^{(k)} = \begin{bmatrix} u_i \\ g_i \\ S_i \\ 0 \end{bmatrix}, \quad \Psi_{ij} = \Psi(\|x_i - \xi_j\|)$$

The value of u(x) close to k can be written in terms of the reconstruction vector as $u^{(k)} = H(x)^{(k)}\alpha^{(k)}$ where the Reconstruction vector

$$H(x)^{(k)} = \left[\Psi(\|\mathbf{x} - \xi_\mathbf{j}\|), B_\xi[\Psi(\|\mathbf{x} - \xi_\mathbf{j}\|)], \bar{L}_\xi[\Psi(\|\mathbf{x} - \xi_\mathbf{j}\|)], P_{m-1} \right]^T$$

Similarly, any PDE operator can be applied to the reconstruction vector $H^{(k)}$ to reconstruct partial derivatives
By applying the linear PDE operator L[ ] to $H^{(k)}$ at the local system centre point, a relation is obtained by linking the values of u_i in the local system. That is,

$$\begin{aligned} S_{centre} &= \bar{L}[u^{(k)}(x_{centre})] = \bar{L}[H^{(k)}(x_{centre})]\alpha^{(k)} \\ &= \left[\bar{L}_x[\Psi(x_{centre} - \xi_j)], \bar{L}_x B_\xi[\Psi(x_{centre} - \xi_j)], \bar{L}_x\bar{L}_\xi[\Psi(x_{centre} - \xi_j)] \ \bar{L}_x[P_{m-1} \right]([A^{(k)}]^{-1}d^{(k)}) \\ &= W_{\bar{L}}^{(k)}(x_{centre})d^{(k)} \end{aligned}$$

By applying the above reconstruction to each local system k, a series of N simultaneous equations $Au = B$ are obtained for $u_i, i = 1, 2, ..., N$; where N is the global number of solution centres. These simultaneous equations can be solved for u_i's using any standard solution techniques.

After obtaining the solution of the global linear system $Au = B$, and using the current interpolation matrix systems and updated data vectors, a reconstruction of $\hat{L}[u^n]$ at Solution and PDE centres are formed for calculating $S(x) = \hat{L}[u^{n-1}] + \Delta t S'(x)$ at the next time step.

The reconstruction array is given by

$$\hat{L}[u^n(x)] = \hat{L}[H^{(k)}(x_{centre})]\alpha^{(k)}$$

$$= \left[\hat{L}_x[\Psi(x - \xi_j)], \hat{L}_x B_\xi[\Psi(x - \xi_j)], \hat{L}_x\bar{L}_\xi[\Psi(x - \xi_j)], \hat{L}_x[P_{m-1}] \right]([A^{(k),n}]^{-1}d^{(k),n}) = W_{\hat{L}}^{(k)}(x)d^{(k)}$$

If the modified PDE operator $\bar{L}$ changes with time, then the local system matrices must be re-formed and re-inverted at each time step

3. Upwind Scheme

For convective dominant problems with discontinuities in the flow, spurious oscillations due to dispersive errors are observed in the numerical results when using numerical techniques based on centrally defined interpolation functions. To control these spurious oscillations it is necessary to use upwind interpolation. Upwind interpolation is defined either by upstream points or heavily weighted on those points. The Upwind scheme proposed in this paper includes the usual RBF based LHI with PDE centres along with central stencil for source centres and upstream stencil of PDE centres.

Using the Upwind scheme unsteady benchmark problems are solved and the solutions are compared with the corresponding solutions of central RBF scheme based LHI with PDE centres, exact values and presented.

4. Solution of Benchmark Problems

- An unsteady homogeneous problem is given by

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x_i^2} - u_i\frac{\partial \phi}{\partial x_i} \qquad 0 \le x \le 1.0; \quad 0 \le y \le 0.2; \quad 0 \le z \le 0.2 \tag{1}$$

with

$$u = (1, 0, 0)^T; \quad \phi(x = 0, t) = 2.0; \quad \phi(x > 0, t = 0) = 1.0$$

The BCs and ICs are taken from the exact solution $\phi(x,t) = 1.0 + \frac{1}{2}(erfc(\frac{x-t}{2\sqrt{Dt}}) + e^{\frac{x}{D}} erfc(\frac{x-t}{2\sqrt{Dt}})$
The comparison of the RMS error values for the problem with the two approaches are presented in Table 1 for different diffusion coefficients and different nodes. Line graphs of exact and numerical solutions at the end of 0.5 sec for two typical cases are presented in Figure 1.

Table 1. Comparison of L_2 Errors (Central and Upwind)

Diffusion Coefficient	Method	Number of Nodes 21	41		81	
		Error	Error	Rate of Convergence	Eror	Rate of Convergence
Shape Parameter (c) = 0.2; Total Time (T) = 0.5; θ = 0.5; Δt = 0.001						
0.05	Central	3.10x10^{-3}	2.60x10^{-3}	0.25	2.40x10^{-3}	0.12
	Upwind	3.10x10^{-3}	2.60x10^{-3}	0.25	2.40x10^{-3}	0.12
0.01	Central	6.00x10^{-3}	2.00x10^{-3}	1.58	1.13x10^{-2}	-2.50
	Upwind	6.40x10^{-3}	1.20x10^{-3}	2.42	9.00x10^{-4}	0.42
Shape Parameter (c) = 0.2; Total Time (T) = 0.5; θ = 0.5; Δt = 0.0001						
0.05	Central	3.50x10^{-3}	1.54x10^{-2}	-2.14	1.39x10^{-1}	-3.17
	Upwind	3.30x10^{-3}	2.60x10^{-3}	0.34	9.40x10^{-3}	-1.85
0.01	Central	3.09x10^{-1}	11.56	-5.22	-	-
	Upwind	1.04x10^{-2}	1.34x10^{-2}	-0.37	2.54x10^{-2}	-0.92

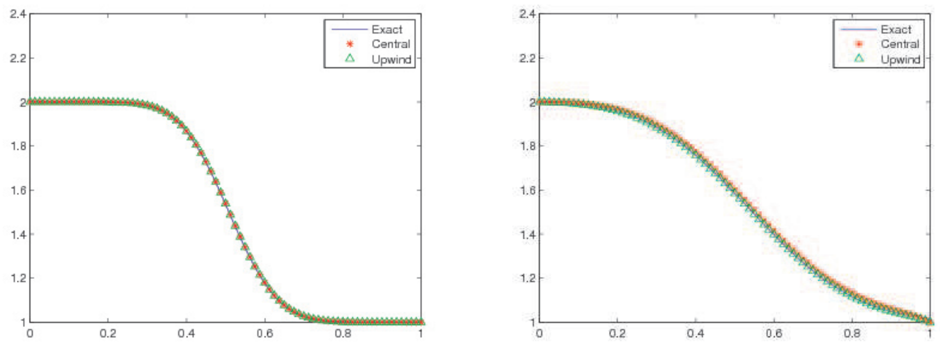

Fig. 1. (N=81, c=0.2, T=0.5, θ=0.5; D=0.01, Δt=0.001 & D=0.05, Δt=0.0001)

- An unsteady equation with non-homogeneous term is given by

$$\frac{\partial u}{\partial t} + a_1\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = f(x), \qquad 0 \le x \le 2.0; \quad t \ge 0 \tag{2}$$

The BCs and ICs are taken from the exact solution which is given by $u(x,t) = \frac{1}{4t+1}e^{-\frac{(x-a_1 t-0.5)^2}{D(4t+1)}}$

The comparison of the RMS error values for the problem with the two approaches are presented in Table 2 and line graphs of exact and numerical solutions at the end of 1.25 sec for two typical cases are presented in Figure 2.

Table 2. Comparison of L_2 Errors (Central and Upwind)

Diffusion Coefficient	Method	Number of Nodes 21	41		81	
		Error	Error	Rate of Convergence	Error	Rate of Convergence
Shape Parameter (c) = 0.2; Total Time (T) = 1.25; a_1 = 0.8; θ = 0.5; Δt = 0.001						
0.01	Central	$1.22x10^{-2}$	-	-	$8.00x10^{-3}$	-
	Upwind	$1.26x10^{-2}$	$2.10x10^{-3}$	2.58	$3.00x10^{-4}$	2.81
0.005	Central	$2.37x10^{-2}$	$6.80x10^{-3}$	1.80	-	-
	Upwind	$1.90x10^{-2}$	$3.00x10^{-3}$	2.66	$3.00x10^{-4}$	3.32
0.001	Central	$1.01x10^{-1}$	$2.97x10^{-2}$	1.76	$4.20x10^{-3}$	2.82
	Upwind	$8.55x10^{-2}$	$1.06x10^{-2}$	3.01	$3.20x10^{-3}$	1.73
Shape Parameter (c) = 0.2; Total Time (T) = 1.25; a_1 = 0.8; θ = 0.5; Δt = 0.0001						
0.01	Central	$1.21x10^{-2}$	-	-	$7.52x10^{-2}$	-
	Upwind	$1.28x10^{-2}$	$2.20x10^{-3}$	2.54	$4.00x10^{-4}$	2.46
0.005	Central	$2.38x10^{-2}$	$6.80x10^{-3}$	1.81	-	-
	Upwind	$1.92x10^{-2}$	$3.00x10^{-3}$	2.68	$4.00x10^{-4}$	2.91
0.001	Central	$1.01x10^{-1}$	$2.93x10^{-2}$	1.79	$2.05x10^{-2}$	0.52
	Upwind	$8.60x10^{-2}$	$1.08x10^{-2}$	2.99	$3.30x10^{-3}$	1.71

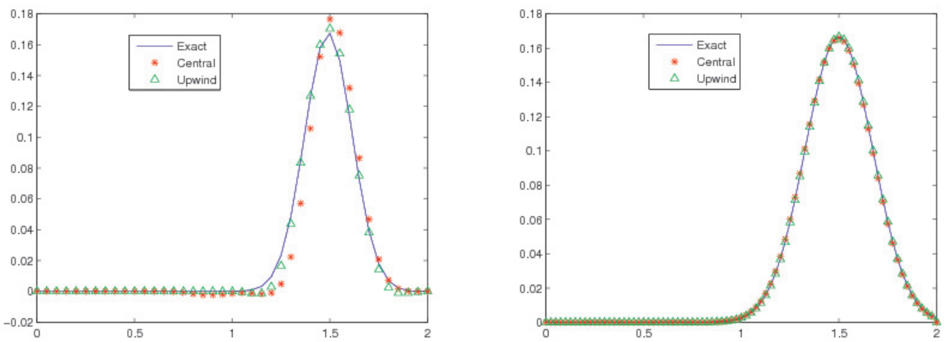

Fig. 2. (c=0.2, T=1.25, a_1=0.8, θ=0.5; N=41, D=0.005, Δt=0.01 & N=81, D=0.01, Δt=0.001)

5. Conclusion

In this paper an Upwind scheme is proposed in the RBF based LHI interpolation with PDE centres. The series of developments in the RBF based approaches leading to the upwind scheme is explained. Formulation of the method for unsteady problems is described. Steady formulation is a part of the unsteady formulation. The upwind approach is applied to some of the unsteady benchmark problems. The addition of upwind stencil for the PDE centres improved the performance of the RBF based LHI method and given better solution for the benchmark problems.

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