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ON THE SOLUTION OF DIFUSION-CONVECTION PROBLEMS BY MEANS OF RBF APPROXIMATIONS

Marcelo J. Colaço
Military Institute of Engineering
Department of Mechanical Engineering
Pç Gen. Tibúcio, 80, Rio de Janeiro, RJ, 22290-270, Brazil
colaco@ime.eb.br

Helcio R. B. Orlande
Federal University of Rio de Janeiro
Department of Mechanical Engineering
Cx. Postal 68503, Rio de Janeiro, RJ, 21945-970, Brazil
helcio@mecanica.coppe.ufrj.br

Nilson C. Roberty
Federal University of Rio de Janeiro
Department of Nuclear Engineering
Cx. Postal 68503, Rio de Janeiro, RJ, 21945-970, Brazil
nilson@con.ufrj.br

Carlos Alves
Instituto Superior Técnico
Department of Mathematics
Av. Rovisco Pais, 1049-001, Lisboa Codex, Portugal
calves@math.ist.utl.pt

Vitor Leitão
Instituto Superior Técnico
Department of Civil Engineering
Av. Rovisco Pais, 1049-001, Lisboa Codex, Portugal
vitor@civil.ist.utl.pt

Abstract. *In this work we use the Kansa's Method, also known as Radial Basis Functions Collocation Method to solve diffusive problems, like steady-state heat transfer and also convective-diffusive problems, like the incompressible steady-state Navier-Stokes equations. No pressure-velocity schemes neither the so called artificial compressibility scheme are used. Also, no interpolation function is needed for the convective terms. In fact, the solution of the original problem is reduced to the solution of a simple system of algebraic equations. Test-cases of practical interest are examined in the paper.*

Keywords. *Meshless Methods, RBF, Linear Heat Conduction, Forced Convection*

1.Introduction

The recent advances in computer technology have provided powerful tools for the simulation of natural phenomenon. Numerical schemes such as finite volume method, finite difference method and the finite element method becomes very popular among them, as they have been studied from its numerical aspects and widely used in various areas. Their success mainly relies on the mesh of good quality. Thus, mesh generation often challenge the numerical simulations associated with industrial and environmental applications, especially for those problems with complex geometry.

Recent development in the automatic mesh generation techniques for mesh-based methods relieves the difficulties. However, to maintain detailed structural information about the computational mesh is still expensive. These make mesh generation, modification, and re-meshing a very complicated task for programmers, mathematicians and engineering.

To overcome the above mentioned difficulties, mesh-free and meshless methods are been developed. Seeking to avoid the drawbacks or weakness of the standard numerical methods, and yet preserving the ability to accommodate geometric complexity. From the viewpoint of kernel interpolation/approximation techniques, many mesh-free methods are based on the moving least square technique. This group of mesh-free methods has been successfully applied to many practical but difficult problems in engineering that are to be solved by the traditional mesh-based methods.

One of the most popular mesh-free kernel approximation technique is radial basis functions (RBFs). Initially, RBFs were developed for multivariate data and function interpolation. It was found that RBFs were able to construct an interpolation scheme with favorable properties such as high efficiency, good quality and capability of dealing with scattered data, especially for higher dimension problems. It is well-known that a good interpolation scheme also has great potential for solving partial differential equations. It was Kansa who made the first step forward in employing RBFs to deal with PDEs. He proposed a simple collocation method using RBFs.

In the present study, the same RBF are used to interpolated velocity and pressure in a two-dimensional Pouiseulle flow without heat transfer numerical experiment. In the second part of the paper, a RBF approximated solution is tested against an analytical solution for a laminar thermally developing flow inside a parallel plate channel.

2. RBF Background

Radial basis functions are essential ingredients of the techniques generally known as "meshless methods". In a way or another all meshless techniques require some sort of radial function to measure the influence of a given location on another part of the domain.

The use of radial basis functions (RBF) followed by collocation, a technique first proposed by Kansa (Kansa, 1990), after the work of Hardy (Hardy, 1971) on multivariate approximation, is now becoming an established approach and various applications to problems of structures and fluids have been made in recent years – see, for example Leitão (Leitão, 2001; Leitão, 2004).

Kansa's method (or asymmetric collocation) starts by building an approximation to the field of interest (normally displacement components) from the superposition of radial basis functions (globally or compactly supported) conveniently placed at points in the domain (and, or, at the boundary).

The unknowns (which are the coefficients of each RBF) are obtained from the (approximate) enforcement of the boundary conditions as well as the governing equations by means of collocation. Usually, this approximation only considers regular radial basis functions, such as the globally supported multiquadrics or the compactly supported Wendland (Wendland, 1998) functions.

Radial basis functions (RBFs) may be classified into two main groups:

1. the globally supported ones namelly the multiquadric (MQ, $\sqrt{\left(x-x_j\right)^2+c_j^2}$, where c_j is a shape parameter), the inverse multiquadric, thin plate splines, guassians, etc;
2. the compactly supported ones such as the Wendland (1998) family (for example, $(1-r)_+^n + p\left(r\right)$ where $p(r)$ is a polynomial and $(1-r)_+^n$ is 0 for r greater than the support).

In a very brief manner, interpolation with RBFs may take the form:

$$s\left(x_i\right)=f\left(x_i\right)=\sum_{j=1}^{N}\alpha_j\phi\left(\left|x_i-x_j\right|\right)+\sum_{k=1}^{\hat{N}}\beta_k p_k\left(x_i\right) \tag{1}$$

where $f(x_i)$ is known for a series of points x_i and $p_k(x_i)$ is one of the $\hat{N}$ terms of a given basis of polynomials, see Buhmann (Buhmann, 2003). This approximation is solved for the α_j unknowns from the system of N linear equations, subject to the conditions (for the sake of uniqueness) $\sum_{j=1}^{N}\alpha_j p_k\left(x_j\right)=0$.

By using the same reasoning it is possible to extend the interpolation problem to that of finding the approximate solution of partial differential equations. This is made by applying the corresponding differential operators to the radial basis functions and then to use collocation at an appropriate set of boundary and domain points.

In short, the non-symmetrical collocation is the application of the domain and boundary differential operators *LI* and *LB*, respectively, to a set of *N-M* domain collocation points and *M* boundary collocation points.

From this, a system of linear equations of the following type may be obtained

$$\begin{aligned} LIu_h\left(x_i\right)&=\sum_{j=1}^{N}\alpha_j LI\phi\left(\left|x_i-\varepsilon_j\right|\right)+\sum_{k=1}^{\hat{N}}\beta_k LIp_k\left(x_i\right)\\ LBu_h\left(x_i\right)&=\sum_{j=1}^{N}\alpha_j LB\phi\left(\left|x_i-\varepsilon_j\right|\right)+\sum_{k=1}^{\hat{N}}\beta_k LBp_k\left(x_i\right)\end{aligned} \tag{2.a,b}$$

subject to the conditions $\sum_{j=1}^{N}\alpha_j p_k\left(x_j\right)=0$ where the α_j and β_k unknowns are determined from the satisfaction of the domain and boundary constraints at the collocation points.

3. Numerical Examples

In this paper, we used the Kansa's Method to solve two different sample problems dealing with convection-diffusion equations. The main purpose of this section is to compare the results obtained through the RBF approximations with the benchmark solutions of these problems found in the literature.

3.1. Pouiseulle Flow

In this section, we will present the approximate results obtained by the RBF expansion for the hydrodynamically developing flow, without heat transfer, within a parallel plate channel with length L and weight h. The mathematical formulation for this problem is given by the mass, x-momentum and y-momentum conservation equations

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \quad \text{in } 0<x<L;\ 0<y<h \tag{3.a}$$

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=\frac{\mu}{\rho}\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)-\frac{1}{\rho}\frac{\partial P}{\partial x} \quad \text{in } 0<x<L;\ 0<y<h \tag{3.b}$$

$$u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=\frac{\mu}{\rho}\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)-\frac{1}{\rho}\frac{\partial P}{\partial y} \quad \text{in } 0<x<L;\ 0<y<h \tag{3.c}$$

subjected to the following boundary conditions

$$u=u_0 \quad \text{at } x=0;\ 0<y<\text{h} \tag{4.a}$$

$$v=0 \quad \text{at } x=0;\ 0<y<h \tag{4.b}$$

$$u=v=0 \quad \text{at } y=0 \text{ and } y=h;\ 0<x<L \tag{4.c}$$

where no boundary condition is assumed to $x=L$; $0<y<h$. Classical numerical methods, like the Finite Volume Method and the Finite Difference Method need to use some kind of pressure-velocity coupling scheme, like the SIMPLEC (Van Doormaal and Raithby, 1984), in order to obtain velocity fields in the x and y-momentum equations that satisfies the mass conservation equation. Also, the convective terms are usually treated by some sort of hybrid or upwind method, like the WUDS (Raithby and Torrance, 1974) and the UTOPIA (Leonard et al, 1995). In this section, instead, we will expand the variables u, v and P by using the following expressions

$$u(x,y)=\sum_{i=1}^{N}\phi_i\psi(\mathbf{r}_i) \tag{5.a}$$

$$v(x,y)=\sum_{j=1}^{N}\phi_j\psi(\mathbf{r}_j) \tag{5.b}$$

$$P(x,y)=\sum_{k=1}^{N/\partial\Omega}\phi_k\psi(\mathbf{r}_k) \tag{5.c}$$

where the functions ψ are the same for the three expansions, but the parameters ϕ are different for each one. Also, the number N and the locations $\mathbf{r}$ of the centers are the same for the u and v expansions. The expansion for the pressure doesn't include the boundary of the domain, since this would imply in an over-specified condition. In other words, if one specify the velocity at the entrance, there is no need to specify also the pressure.

Using Eqs. (5) into Eqs. (3) and (4) we obtain

$$\sum_{i=1}^{N}\phi_i\frac{\partial\psi_i}{\partial x}+\sum_{j=1}^{N}\phi_j\frac{\partial\psi_j}{\partial x}=0 \quad \text{in } 0<x<L;\ 0<y<h \tag{6.a}$$

$$\left(\sum_{i=1}^{N}\phi_i\psi_i\right)\left(\sum_{i=1}^{N}\phi_i\frac{\partial\psi_i}{\partial x}\right)+\left(\sum_{j=1}^{N}\phi_j\psi_j\right)\left(\sum_{i=1}^{N}\phi_i\frac{\partial\psi_i}{\partial y}\right)=\frac{\mu}{\rho}\left(\sum_{i=1}^{N}\phi_i\frac{\partial^2\psi_i}{\partial x^2}+\sum_{i=1}^{N}\phi_i\frac{\partial^2\psi_i}{\partial y^2}\right)-\frac{1}{\rho}\sum_{k=1}^{N/\partial\Omega}\phi_k\frac{\partial\psi_k}{\partial x} \quad \text{in } 0<x<L;\ 0<y<h \tag{6.a}$$

$$\left(\sum_{i=1}^{N}\phi_i\psi_i\right)\left(\sum_{j=1}^{N}\phi_j\frac{\partial\psi_j}{\partial x}\right)+\left(\sum_{j=1}^{N}\phi_j\psi_j\right)\left(\sum_{j=1}^{N}\phi_j\frac{\partial\psi_j}{\partial y}\right)=\frac{\mu}{\rho}\left(\sum_{j=1}^{N}\phi_j\frac{\partial^2\psi_j}{\partial x^2}+\sum_{j=1}^{N}\phi_j\frac{\partial^2\psi_j}{\partial y^2}\right)-\frac{1}{\rho}\sum_{k=1}^{N/\partial\Omega}\phi_k\frac{\partial\psi_k}{\partial x} \quad \text{in } 0<x<L;\ 0<y<h \tag{6.a}$$

$$\sum_{i=1}^{N}\phi_i\psi_i=u_0 \quad \text{at } x=0;\ 0<y<h \tag{7.b}$$

$$\sum_{i=1}^{N} \phi_j \psi_j = 0 \qquad \text{at } x=0;\ 0<y<h \tag{7.b}$$

$$\sum_{i=1}^{N} \phi_i \psi_i = \sum_{i=1}^{N} \phi_j \psi_j = 0 \qquad \text{at } y=0 \text{ and } y=h;\ 0<x<L \tag{7.c}$$

which results in a non-linear system for ϕ_i, ϕ_j and ϕ_k that can be solved by a quasi-Newton method. Note that no pressure-velocity coupling neither an upwind method was used.

For this comparison, we considered water at 20 °C, with the following physical properties: ρ=1000.52 kg/m^3, μ=0.001 kg/m.s. The height of the channel was taken as 0.05 m and the mean velocity was taken as 0.001 m/s, which gives a Reynolds number equal to 100. In order to validate the results with an analytical solution, the length of the channel was taken in order to have a fully developed flow. According to Bodoia and Osterle (1961), such length is given as

$$\frac{L}{2h\,\mathrm{Re}} = 0.0110 \tag{8.a}$$

which results in L=0.11 m. For the fully developed flow, the velocity profile is given as

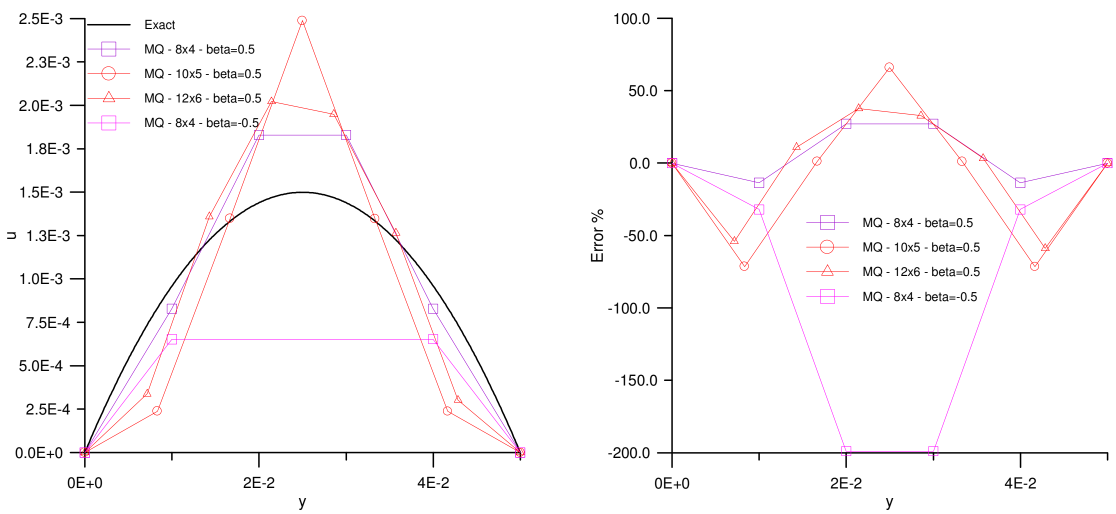
$$u(y) = -\frac{6u_{av}}{h^2}\left(y^2 - hy\right) \tag{8.b}$$

where u_{av} is the average velocity along the y-direction and v is zero everywhere.

Figure (1) shows the results obtained by using a multiquadrics function given by

$$\phi_i(x,y) = \left[(x-x_i)^2 + (y-y_i)^2 + c_i^2\right]^{\beta} \tag{9}$$

where the exponent β was varied and the parameter c was automatically obtained by the minimization of the mean square root of the residual of Eqs. (6) and (7). Note the large discrepancy of the results, when comparing the percentual errors appearing in Fig. (1.b).



(a) (b)

Figure 1. Results using the multiquadrics approximation

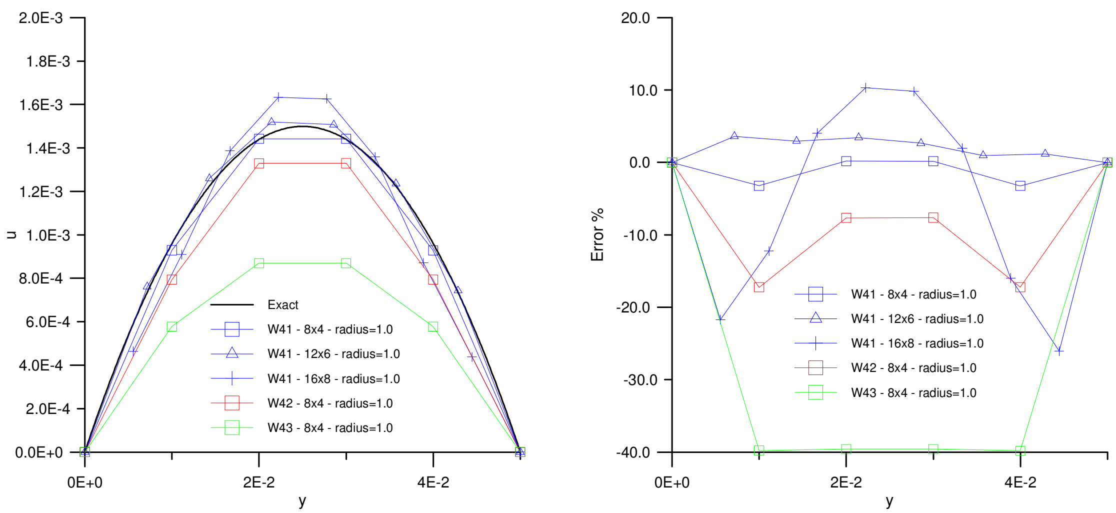
Figure (2) shows the results obtained by using Wendland functions given by

$$\text{W41:}\quad \phi_i(x,y) = \left(\sqrt{(x-x_i)^2+(y-y_i)^2} - 1\right)_+^4 \left(1 + 4\sqrt{(x-x_i)^2+(y-y_i)^2}\right) \tag{10.a}$$

$$\text{W42:}\quad \phi_i(x,y) = \left(\sqrt{(x-x_i)^2+(y-y_i)^2} - 1\right)_+^6 \left\{3 + 18\sqrt{(x-x_i)^2+(y-y_i)^2} + 35\left[(x-x_i)^2+(y-y_i)^2\right]\right\} \tag{10.b}$$

$$\text{W43:}\quad \phi_i(x,y)=\left(\sqrt{(x-x_i)^2+(y-y_i)^2}-1\right)_+^8 \left\{1+8\sqrt{(x-x_i)^2+(y-y_i)^2}+25\left[(x-x_i)^2+(y-y_i)^2\right]+32\left[(x-x_i)^2+(y-y_i)^2\right]^{3/2}\right\} \tag{10.c}$$

Note that the solutions are better than those presented in Fig. (1). Also the percentual errors are lower as shown in Fig. (1.b). In all these solutions, the number of expansion points is limited by the ill-conditioness of the problem. Large centers imply in a more ill-conditioned problem. Note, also in Fig. (1.b) that the Wendland function W41 is better than the W42 and W43, for this problem.



(a) (b)

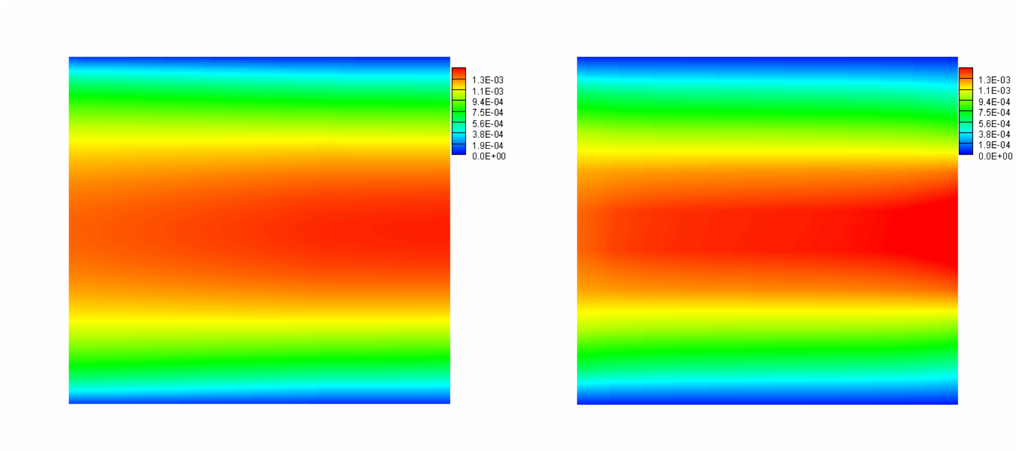
Figure 2. Results using the Wendland approximation

It is quite interesting that the W41 function with only 8x4 centers presented a relative error less than 3 %. Just for comparison, the same problem solved by the Finite Volume Method, using the SIMPLEC pressure velocity scheme and the WUDS interpolation scheme with 50x60 grid cells (Colaço, 2001), gives an relative error equal to 1.43 % at y=0.4 mm. This is quite remarkable when one check that this result was obtained only in 0.84 seconds, as showed in Table (1).

Table 1 – Computational time

Type of function	Points in the expansion	Expoent - β	Shape factor - c	Residual - ε	CPU time (seconds)
MQ	8x4	0.5	0.001	8.35 E-5	1.40
		-0.5	0.001	1.76 E-5	1.45
	10x5	0.5	0.0002	1.68 E-5	4.32
	12x6	0.5	0.0005	5.31 E-5	11.11
W41	8x4	N/A			0.84
	10x5				7.38
	12x6				6.06
	16x8				61.93
W42	8x4				1.78
W43					2.91

Finally, Fig. (3) shows the plot of the velocity component u along the entire channel obtained by the W41 approximation with 16x8 points and by the FVM with a 50x60 grid cells (Colaço, 2001). One can see that the W41 expansion gives a reasonable approximation, considering its very low computational cost and the low number of centers.



(a) (b)

Figure 3. Component u of velocity field obtained from the (a) FVM and (b) RBF solutions

3.2. Thermally Developing Flow

In this section, the RBF approximation solution was tested against an analytical solution (Cotta and Özisik, 1986) for a laminar thermally developing flow inside a parallel plate channel with length L and weight h, subjected to a constant heat flux q at the walls. The density ρ, the conductivity k and the specific heat at constant pressure c_p were considered constants, and the mathematical formulation for this steady-state problem is given by the following energy equation

$$u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}=\frac{k}{\rho\, c_p}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right) \quad \text{in } 0<x<L;\ 0<y<h \tag{11.a}$$

subjected to the following boundary conditions

$$T=T_0 \quad \text{at } x=0;\ 0<y<h \tag{11.b}$$

$$k\frac{\partial T}{\partial y}=q \quad \text{at } y=0;\ 0<x<L \tag{11.c}$$

$$-k\frac{\partial T}{\partial y}=q \quad \text{at y}=h;\ 0<x<L \tag{11.d}$$

where the velocity field was considered fully developed. Thus, u has a parabolic distribution given by Eq. (8.b)

The temperature T can be written as an RBF expansion over N centers distributed over the entire domain, including the boundaries. Note that in this approach there is no need to use an upwind scheme, since the derivatives of T are obtained directly from the following equation.

$$T(x,y)=\sum_{i=1}^{N}\phi_i\psi(\mathbf{r}_i) \tag{12}$$

where $\mathbf{r}_i$ is the distance between the point (x,y) and the center (x_i,y_i).

Thus, applying Eq. (12) to Eqs. (11.a)-(11.d) we obtain

$$u\sum_{i=1}^{N}\phi_i\frac{\partial\psi(\mathbf{r}_i)}{\partial x}+v\sum_{i=1}^{N}\phi_i\frac{\partial\psi(\mathbf{r}_i)}{\partial y}=\frac{k}{\rho\, c_p}\left[\sum_{i=1}^{N}\phi_i\frac{\partial^2\psi(\mathbf{r}_i)}{\partial x^2}+\sum_{i=1}^{N}\phi_i\frac{\partial^2\psi(\mathbf{r}_i)}{\partial y^2}\right] \quad \text{in } 0<x<L;\ 0<y<h \tag{13.a}$$

$$\sum_{i=1}^{N}\phi_i\psi(\mathbf{r}_i)=T_0 \quad \text{at } x=0;\ 0<y<h \tag{13.b}$$

$$k\sum_{i=1}^{N}\phi_i\frac{\partial\psi(\mathbf{r}_i)}{\partial y}=q \quad \text{at } y=0;\ 0<x<L \tag{13.c}$$

$$-k\sum_{i=1}^{N}\phi_i \frac{\partial \psi(\mathbf{r}_i)}{\partial y} = q \quad \text{at } y=h;\ 0<x<L \tag{13.d}$$

or, in matricial form

$$\mathbf{\Psi\Phi} = \boldsymbol{\beta} \tag{14}$$

where $\mathbf{\Psi}$ is the matrix of the RBF functions and their derivatives, $\mathbf{\Phi}$ is the vector of the unknown parameters and $\boldsymbol{\beta}$ is the RHS of the equations. Since the velocity field is known, the problem is linear.

The analytical solution of this problem was obtained by Cotta and Özisik (1986) and it was given in terms of the Nusselt number at the top surface of the channel as a function of the non-dimensional axial length, which are given as

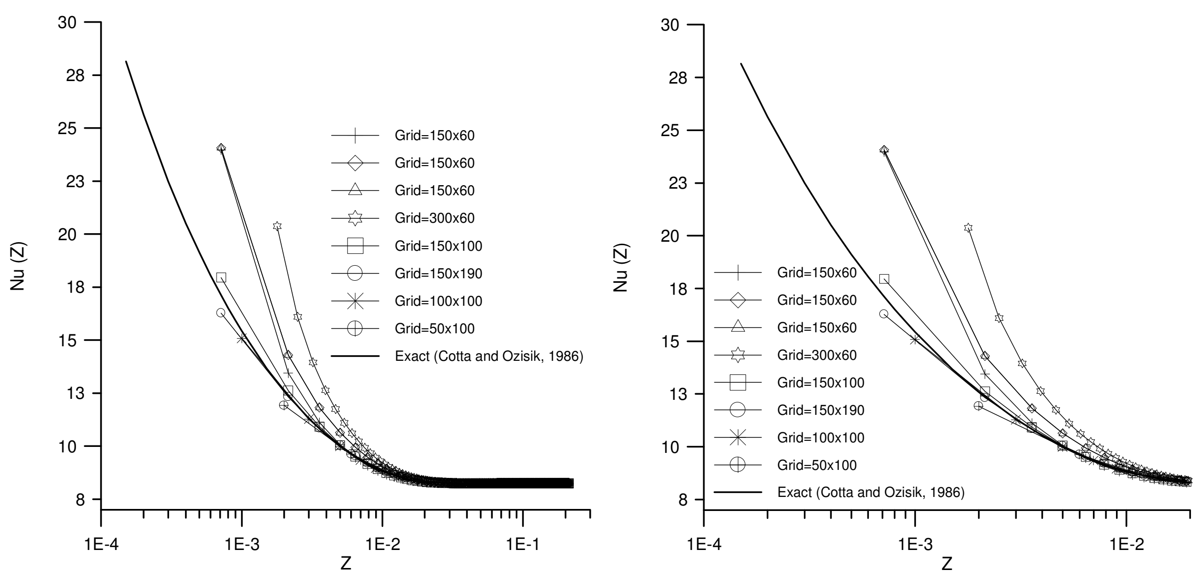
$$Nu(Z) = \frac{2hq}{k[T(x,y=h)-T_{av}(x)]}; \quad Z = \frac{(k/\rho c_p)x}{4u_{av}h^2} \tag{15.a,b}$$

where u_{av} is the mean velocity in the x direction and T_{av} is the average temperature, defined as

$$T_{av} = \frac{\int_0^h u(x,y)T(x,y)dy}{u_{av}h} \tag{16}$$

For this comparison, we considered water at 20 °C, with the following physical properties: ρ=1000.52 kg/m^3, k=0.597 W/m.K, c_p=4.1818 KJ/kg.°C. The height of the channel was taken as 0.05 m and the length as 1 m. The mean velocity was taken as 0.001 m/s, which gives a Reynolds number equal to 100. Notice that the total length is not large enough to have the flow fully thermally developed. According to the results of Cotta and Özisik (1986), the total length should be approximately equal to 7 m. However, we are interested only in the portion close to the entrance, where the variation of the Nusselt number is very large.

Figure (4.a) shows the results obtained by Colaço (2001) using the Finite Volume Method, with a WUDS scheme for the convective terms, for a length equal to 7 m and Figure (4.b) shows the same graphic for $0<x<1$.



(a) (b)

Figure 4. Results using the Finite Volume Method (Colaço and Orlande, 2001)

Note, from Fig. (4), that all grids are capable of estimate the Nusselt number at the fully developed region, but there are large discrepancies close to the entrance. In fact, the better results are obtained by using 100x100 and 150x190 grid cells.

In Fig. (5) the MQ results were obtained by using the multiquadrics expression given by Eq. (9). The W4x expansions were defined by using the Wendland compact form as showed in Eqs. (10.a)-(10.c)

Figure (5.a) shows very poor results when using β=0.5 for 80x4, 100x5 and 120x6 grid points. Although the solution by RBF's doesn't require a uniform distribution of points, we choose a uniform distribution in order to compare with the results presented in Fig. (4). We also tried the Wendland's function for this test case, but the results were very poor, as one can see from Fig. (5.a).

Note, in Fig. (5.b), the great improvement in the solution when we used β = -0.5 for the 120x6 expansion, when compared with β = 0.5 from Fig. (5.a). Also, other values of β show better results than those from Fig. (5.a). Figure (5.c) shows the results for a 140x7 expansion, when the results are even better, although still far away from the analytical solution from Cotta and Özisik. It is interesting to note the small number of points in the *y*-direction for all test cases.

Also, Fig. (5.d) shows the results obtained through the RBF, when compared with those obtained by the Finite Volume Method. It is very interesting to note the dependency of the FVM solution with the number of points in the *y* direction as one can see by comparing the results obtained by using 150x60 with 60x100 grid cells. This fact doesn't occur with the RBF solutions.

It is worth to mention that the better RBF solution is still very poor when compared with the better FVM solution. In fact, when one tries to increase the number of centers in the RBF approximation beyond the ones presented in the Fig. (5), the system becomes too ill-conditioned to solve and no physical solution is obtained. Also, all the RBF solutions presented here were obtained after a proper choice of the shape parameter *c*, appearing in Eq. (9). Such choice was made in order to minimize the residual of the Eq. (14), defined as:

$$\varepsilon = \left\| \mathbf{\Psi\Phi} - \boldsymbol{\beta} \right\| \tag{17}$$

where ||.|| denotes the Euclidian norm of the vector.

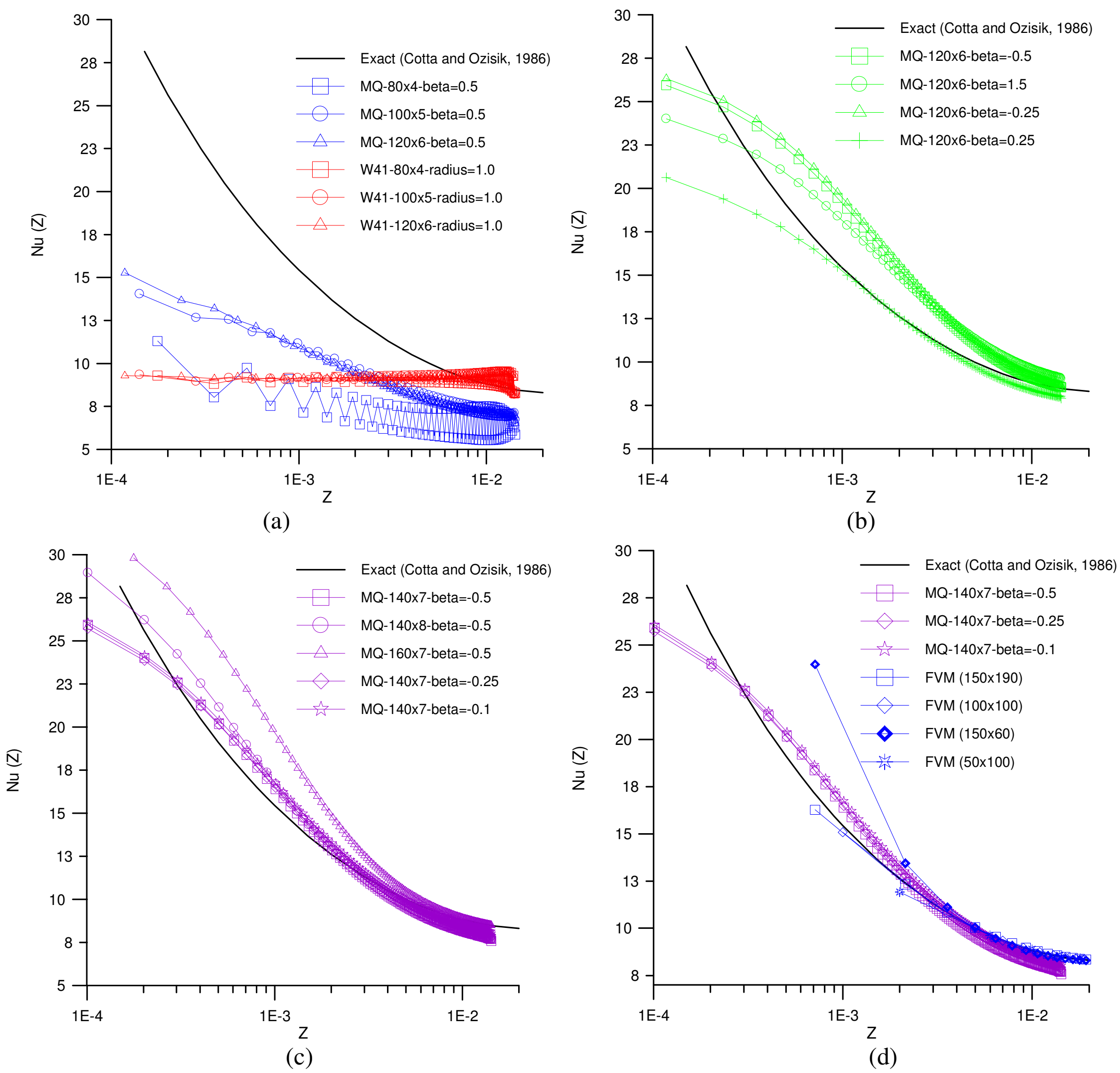
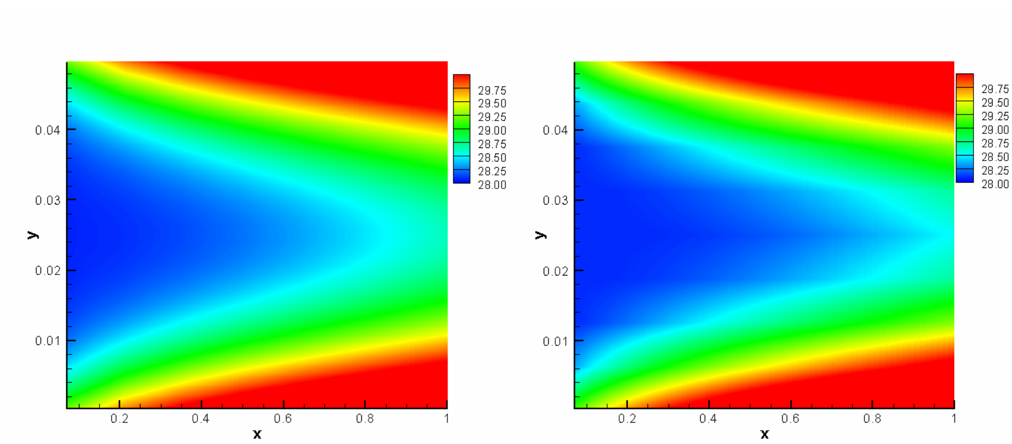


Figure 5. Results using the RBF expansion

Finally, Table (2) presents the shape parameter used in each one of the expansion, as well as the CPU time in seconds (in an Intel Centrino 1.5 GHz with 1.5 Gb RAM) and the value of the residual ε. While the RBF results presented in Fig. (5) don't present a very good accuracy, when compared with the analytical solution, the execution time obtained in their solution is very small (less than 2 seconds) and they can used as an estimative of the correct answer. Also, if better solvers for the linear system were used and a better choice of the shaper parameter c or the exponent β was employed, better results could be obtained. Note also that the general temperature field is similar for the two methods, as one can see in Fig. (6) for the FVM with 100x100 grid cells (Colaço, 2001) and for the RBF with 140x7 points. The sharpness of the RBF solution is due to the lack of points in the *y*-direction (only 7 against 100 in the FVM).

Table 2 – Results from the RBF expansion

Points in the expansion	Shape parameter - c	Expoent - β	Residual - ε	CPU time (seconds)
80x4	0.003	0.5	7495	0.08
120x6	0.043	-0.5	1295	0.81
	0.011	1.5	41049381	0.79
	0.043	-0.25	1185	0.88
	0.015	0.25	8564	0.78
	0.004	0.5	2311	0.83
100x5	0.006		9790	0.33
140x7	0.024	-0.5	9614	1.96
	0.021	-0.25	2504	1.98
	0.001	0.5	44736	1.96
	0.020	-0.1	3084	1.98
140x8	0.023	-0.5	5158	2.6
160x7	0.038		6575	2.9



(a) (b)

Figure 6. Temperature field obtained from the (a) FVM and (b) RBF solutions

4. Acknowledgements

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