Journal of Mathematical Modeling
Vol. 11, No. 1, 2023, pp. 71–81. Research Article

JMM

A new approximation method for convection-diffusion equation by the fundamental solutions

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Abstract. This paper develops a new numerical method of fundamental solutions for the non-homogeneous convection-diffusion equations with time-dependent heat sources. A summation of the fundamental solutions of the diffusion operator is considered with time-dependent coefficients for the solution of the underlying problem. By the θ-weight discretiztion for the time derivative and selecting the source points and the field points at each time level, the solutions of all time levels are obtained. In addition, the stability of this approach is analyzed by considering $\theta = 1$ in numerical results. This method is truly meshless and it is not necessary to discretize any part of the domain or boundary. As a result, this method is easily applicable to higher dimensional problems with irregular domains. In this work, we consider a non-homogeneous convection-diffusion equation (NCDE) in 2D with a regular domain and present some numerical results to show the effectiveness of the proposed method.

Keywords: Non-homogeneous diffusion equations, meshfree method, method of fundamental solutions, time-dependent fundamental solutions.
AMS Subject Classification 2010: 34A34, 65L05.

1 Introduction

Solving problems with regular domains by mesh-dependent methods such as finite difference method (FDM) and finite element method (FEM) is easy and efficient. However, as they are mesh-dependent, their applicability become difficult especially in the case of 3D and higher dimensional problems.

However, in the boundary element method (BEM) the discretization is required only on the boundary and the shape complexity of the domain does not matter. Instead, evaluation of the domain integrals in the source term and singular integrals related to fundamental solutions (FS) [19] require significant

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Received: 20 May 2022 / Revised: 2 December 2022 / Accepted: 27 December 2022
DOI: 10.22124/JMM.2022.22266.1968

computational efforts. For several decades, the meshfree and integration free approaches have been used to solve the partial differential equations (PDEs) to overcome these difficulties [3, 14, 21].

Thereinafter, the Trefftz method (TM) is used by a linear combination of Trefftz basis functions to approximate the solution of PDE [7]. One of the main categories of these functions is known as F-Trefftz and is also called the method of fundamental solutions (MFS). This method is based on the FS of the intended differential operator [9, 12]. The MFS is used when the FS of PDE or a part of that is known and that is exactly what is done in the BEM. This method is simple and, due to its meshfree property, we can easily get numerical solutions of linear elliptic PDEs [9]).

The MFS was initially used to solve the elliptic equations, such as Laplace and Helmholtz equation [9, 15, 18] and to approximate the solution of parabolic-type PDEs like diffusion equation [11, 28]. Later on, the MFS was extended to time-dependent problems to solve homogeneous or non-homogeneous types by a few methods such as time-marching MFS [25], the unified time-space MFS with diffusion FS [28] or eigenfunction expansion MFS [30]. By mixing the MFS with other approaches namely the method of particular solution (MPS) [1, 11, 17, 23, 29] and the dual reciprocity method (DRM) [2, 5, 8, 22, 31], various types of non-homogeneous equations can be solved. In these methods, the MFS is used to the part of equation that satisfies FS and MPS or DRM are applied to the remaining part of the equation. The MFS with modified Helmholtz FS was applied to a diffusion problem with boundary conditions of Dirichlet-type in [11]. Also, Young et al. solved a homogeneous diffusion equation by using diffusion FS bases directly [28]. Furthermore, solving non-homogeneous diffusion problems is possible by using diffusion FS for homogeneous part of the problem and DRM approach for the non-homogeneous source term [29].

In this work, we have applied MFS introduced by Young et al. to obtain the non-homogeneous diffusion solution by a time-dependent heat source [28] and FS of the diffusion equation is considered as the basis functions to the solution of the whole equation. Unlike the previous attempts such as [10, 19, 27, 29], in this approach, using a particular solution or the Laplace transform is not required to overcome the non-homogeneous part of the problem. As a result, the computational costs can be considerably saved. In addition, we have used the Tikhonov regularization technique [26] to obtain the solution of the resulting system of equations that can be an ill-conditioned problem [6, 24].

The rest of work is organized as follows. The convection-diffusion problem is introduced in Section 2. In Section 3, an extension of the MFS with time dependent coefficients is used for NCDE. A new MFS for time discretization is provided in Section 4. Section 5 is devoted to some numerical results for 2D examples. In Section 6, we have stated a brief conclusion and suggested some works for the future.

2 The convection-diffusion problem

We consider the following non-homogenous convection-diffusion equation

$$\frac{\partial u(\boldsymbol{x},t)}{\partial t} - \kappa \triangle u(\boldsymbol{x},t) - \nu \cdot \nabla u(\boldsymbol{x},t) = f(\boldsymbol{x},t), \qquad \boldsymbol{x} \in \Omega \subset \mathbb{R}^d, \quad t > 0, \tag{1}$$

where $\triangle$ and ∇ represent the Laplacian and the gradient operator, respectively, κ is the coefficient of diffusion, ν is a constant vector, and $u(\boldsymbol{x},t)$ may be temperature or concentration for heat or mass transfer. The initial condition of Eq. (1) is as

$$u(\boldsymbol{x},0) = u_0(\boldsymbol{x}), \tag{2}$$

and the boundary condition is given by

$$\mathscr{B}u(\boldsymbol{x},t) = \bar{u}(\mathbf{x},t), \qquad \boldsymbol{x} \in \partial\Omega, \quad t > 0, \tag{3}$$

where $\bar{u}(\mathbf{x},t)$ is a known function, and $\mathscr{B}$ is a boundary operator, which may be of Dirichlet, Neumann or mixed type, and $\partial\Omega$ represents the boundary of Ω. The convection-diffusion problem is combined with diffusion and convection problems, and describes some engineering and physical phenomena that wherein transferred particles, energy or other quantities due to two diffusion and convection processes. Using numerical methods to solve such problems is necessary, even though analytical solutions can be obtained for some cases.

3 An extension of the MFS

This section is devoted to our proposed method that is based on time-dependent FS. We modify the MFS suggested in [28] for solving the linear diffusion problems. As in [28], the time-dependent FS diffusion equation satisfy the following equation

$$\frac{\partial F(\mathbf{x},t;\xi,\tau)}{\partial t} = k\nabla^2 F(\mathbf{x},t;\xi,\tau) + \delta(\mathbf{x}-\xi)\delta(t-\tau), \tag{4}$$

where δ is the Dirac delta function acting at the source point (ξ,τ). This function goes to infinity at $(\mathbf{x},t) = (\xi,\tau)$ and equal to zero elsewhere. The solution of the above equation is determined by using the Fourier transform with respect to $\mathbf{x}$ and the Laplace transform for t as follows

$$F(\mathbf{x},t;\xi,\tau) = \frac{e^{\frac{-|\mathbf{x}-\xi|^2}{4k(t-\tau)}}}{(4k\pi(t-\tau))^{\frac{d}{2}}} H(t-\tau), \tag{5}$$

where d denotes the spatial dimension and $H(t)$ is the Heaviside step function as follows

$$H(t-\tau) = \begin{cases} 1 & t > \tau, \\ 0 & t \leq \tau. \end{cases} \tag{6}$$

By taking $c > max(t-\tau)$ as a constant, the following non-singular homogeneous solution of Eq. (5) can be obtained in the domain

$$G(\mathbf{x},t;\xi,\tau) = F(\mathbf{x},t+c;\xi,\tau).$$

Since the diffusion FS is the solution of the homogenous diffusion equation, we can express the solution of the homogeneous equation in the standard MFS, by a linear combination of the FS of diffusion operator to determine the unknown coefficients considering initial and boundary conditions. In this work, we assume a linear combination of diffusion FS with time-dependent coefficients as the solution of the convection-diffusion problem

$$u(\mathbf{x},t) = \sum_{j=1}^{N_i+N_b} \alpha_j(t) G(\mathbf{x},t;\xi_j,\tau_j), \tag{7}$$

where $\mathbf{x}$ and t are the spatial and the time variables of the field points, ξ_j and τ_j represent the spatial and time coordinates of the source points, and also the number of the initial and boundary source points are

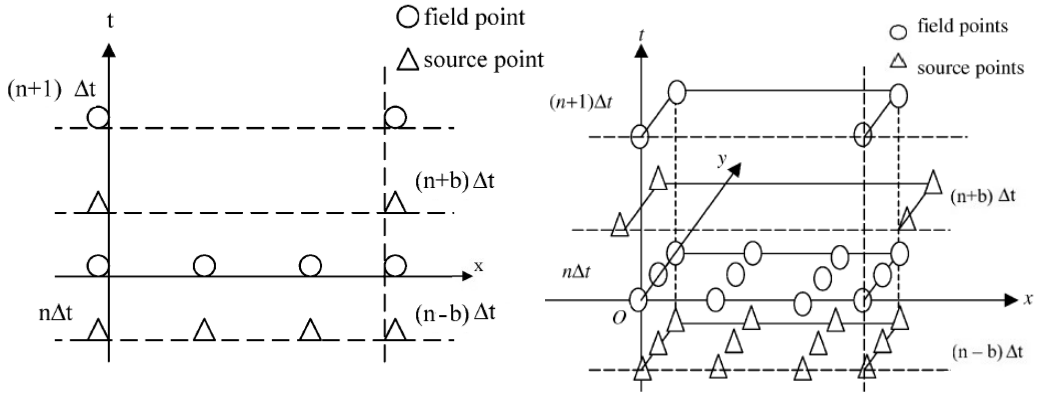

Figure 1: Schematic diagram of source and field points (a) 1-D diffusion and (b) 2-D diffusion problems, $0 < b < 1$ indicates the time levels different form the time steps.

denoted by N_i and N_b, respectively that $N = N_i + N_b$. Moreover, the unknown coefficients $\{\alpha_j(t)\}_{j=1}^{N_i+N_b}$ can be obtained by the collocation method. In some works such as [4, 9, 10], choosing the source points situations has been studied. As shown in Fig. 1 (a) and (b) for 1-D and 2-D, the source points are chosen on different time levels but in the same situation and the field points are located in $t = (n+1)\Delta t$ and $t = n\Delta t$, respectively for the boundary and the interior points.

4 Using the new MFS for NCDE

First, we substitute (7) into the convection-diffusion equation (1) that results,

$$\frac{\partial}{\partial t}\left(\sum_{j=1}^{N}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j)\right) - \kappa\triangle\left(\sum_{j=1}^{N}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j)\right) - \nu\cdot\nabla\left(\sum_{j=1}^{N}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j)\right) = f(\mathbf{x},t). \tag{8}$$

This further can be rewritten as

$$\sum_{j=1}^{N}\frac{\partial}{\partial t}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j) + \sum_{j=1}^{N}\alpha_j(t)\frac{\partial}{\partial t}G(\mathbf{x},t;\xi_j,\tau_j) - \kappa\sum_{j=1}^{N}\alpha_j(t)\triangle G(\mathbf{x},t;\xi_j,\tau_j) - \nu\cdot\sum_{j=1}^{N}\alpha_j(t)\nabla G(\mathbf{x},t;\xi_j,\tau_j) = f(\mathbf{x},t). \tag{9}$$

Since $G(\mathbf{x},t;\xi_j,\tau_j)$ satisfies (4), we can replace the second and third terms of the left hand side of (9) by $\delta(\mathbf{x}-\xi)\delta(t-\tau)$. Now by choosing suitable source points, the above mentioned terms vanish and (9) reduces to

$$\sum_{j=1}^{N}\frac{\partial}{\partial t}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j) - \nu\cdot\sum_{j=1}^{N}\alpha_j(t)\nabla G(\mathbf{x},t;\xi_j,\tau_j) = f(\mathbf{x},t). \tag{10}$$

Using a two-level θ-weighted time scheme, Eq. (10) and the initial and the boundary conditions can be rewritten as

$$\sum_{j=1}^{N}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j) - \theta\nu\cdot\sum_{j=1}^{N}\alpha_j(t)\nabla G(\mathbf{x},t;\xi_j,\tau_j)-(1-\theta)\left(\nu\cdot\sum_{j=1}^{N}\alpha_j(t-\Delta t)\nabla G(\mathbf{x},t;\xi_j,\tau_j)\right)$$
$$=\sum_{j=1}^{N}\alpha_j(t-\Delta t)G(\mathbf{x},t;\xi_j,\tau_j)+\Delta t\, f(\mathbf{x},t), \tag{11}$$

and

$$\sum_{j=1}^{N}\alpha_j(t)G(\mathbf{x},t;\xi_j,\tau_j)=\bar{u}(\mathbf{x},t),\quad \mathbf{x}\in\partial\Omega,\quad t\in(0,t_f). \tag{12}$$

Now suppose that

$$a_{i,j}=\begin{cases}\dfrac{e^{\frac{-|\mathbf{x}_i-\xi_j|^2}{4k(t_i+c-\tau_j)}}}{(4k\pi(t_i+c-\tau_j))^{\frac{d}{2}}}, & \text{if}\quad t_i>\tau_j,\\ 0, & \text{if}\quad t_i\le\tau_j,\end{cases}$$

and let the indexes of internal and boundary points be denoted, respectively, by $\mathfrak{I}$ and $\mathfrak{B}$ and consider $N=N_{\mathfrak{I}}+N_{\mathfrak{B}}$. The matrix A with entries a_{ij} can be written as follows, $A=A_{\mathfrak{I}}+A_{\mathfrak{B}}$, where

$$A_{\mathfrak{I}}=\left[a_{ij}\text{ for }(i\in\mathfrak{I},1\le j\le N)\text{ and 0 elsewhere}\right],$$
$$A_{\mathfrak{B}}=\left[a_{ij}\text{ for }(i\in\mathfrak{B},1\le j\le N)\text{ and 0 elsewhere}\right].$$

Then, Eqs. (11) and (12) can be written in the following matrix form

$$C\boldsymbol{\alpha}^{n+1}=E\boldsymbol{\alpha}^{n}+\boldsymbol{v}^{n+1}, \tag{13}$$

where

$$C=A-\Delta t\theta\nu\cdot\nabla A_{\mathfrak{I}},$$
$$E=A_{\mathfrak{I}}+\Delta t(1-\theta)\nu\cdot\nabla A_{\mathfrak{I}},$$
$$\boldsymbol{v}^{n+1}=\left[\Delta t f^{i,n}\text{ for }(i\in\mathfrak{I})\text{ and }\bar{u}^{j,n+1}\text{ for }(j\in\mathfrak{B})\right]^T,$$
$$\boldsymbol{\alpha}^{n}=(\alpha_1^n,\ \ldots,\alpha_N^n)^T.$$

and $f^{i,n}=f(\mathbf{x}_i,t_n)$ and $\bar{u}^{j,n+1}=\bar{u}(\mathbf{x}_j,t_{n+1})$.

Now by solving Eq. (13) and using initial condition, $\boldsymbol{\alpha}^{n+1}$ can be obtained for the time level n. We start this procedure by solving (2) to find $\alpha_j(0),\ j=1,\ldots,N$ and we proceed it until the solution of final time is achieved.

As mentioned in [20], the coefficient matrices of MFS are often ill-conditioned and solving system (13) can produce unstable results. So, to overcome this difficulty, we can stabilize the solution using Tikhonov regularization method. Let the system be summarized as follows

$$[M_{i,j}]\{\alpha_j\}=\{b_i\}.$$

Using Tikhonov regularization method, we can solve the following system instead, to achieve a well-conditioned problem

$$(M^T M + \lambda I)\alpha = M^T b,$$

where $\lambda > 0$ is the regularization parameter which can be found by trial and error. Note that there are efficient rules for choosing suitable λ, for instance, the L-curve method, which was firstly developed by Lawson and Hansen [13, 16]. In this work, we just check the value of $\lambda > 0$ as the regularization parameter by trial and error.

Now, after using Tikhonov regularization method and obtaining α_j, we can find the solution of time level n by the following matrix multiplication

$$\boldsymbol{u}^n = M\alpha^n.$$

This procedure will be continued until the solutions of all time levels are obtained.

5 Numerical results

To check the validity of the proposed method, two examples of 2-D non-homogeneous convection-diffusion problems with Dirichlet boundary conditions are solved and the numerical results are compared with the exact solutions. To measure the accuracy of the approximate solutions, we use the root mean square error (RMSE), relative error (RE) and the maximum error (ME) as follows

$$RE = \sqrt{\frac{\sum_{j=1}^{N_t}(\hat{u}_j - u_j)^2}{\sum_{j=1}^{N_t}(u_j)^2}}, \quad RMSE = \sqrt{\frac{1}{N_t}\sum_{j=1}^{N_t}(\hat{u}_j - u_j)^2}, \quad ME = \max_{1\le j\le N_t}|\hat{u}_j - u_j|,$$

where $\hat{u}_j$ and u_j are the numerical and exact solutions at the jth node, respectively, and N_t is the number of testing nodes uniformly distributed in the problem domain.

Example 1. Consider the following problem

$$\frac{\partial u(\boldsymbol{x},t)}{\partial t} - \triangle u(\boldsymbol{x},t) - \nabla u(\boldsymbol{x},t) = f(\boldsymbol{x},t),\ t \in (0,t_f),\ \mathbf{x} = (x,y),$$

with the initial condition $u(\mathbf{x},0) = 0$ for $\mathbf{x} \in \Omega$, and the boundary condition

$$u(\mathbf{x},t) = \sin(x)\sin(y)\sin(t), \quad \mathbf{x} \in \partial\Omega, \quad t > 0,$$

where $f(\mathbf{x},t) = \sin x \sin y(\cos t + 2\sin t) - \sin t(\cos x \sin y + \sin x \cos y)$. The analytical solution of the problem is given by $u(\mathbf{x},t) = \sin(x)\sin(y)\sin(t)$.

The results have been obtained for $N_i = 81, N_b = 40$ and in Table 1, the ME, RE and RMSE for $t_f = 1,2,3$ s with different time step sizes are reported. The numerical solution $\hat{u}$ and the absolute error for $\Delta t = 0.05$ and final time $t_f = 3$ are drawn in Fig. 2.

The sensitivity of the solution by choosing the regularization parameter λ has been investigated by numerical results for some different values of λ which shows the effect of the regularization on the quality of the solution given by Eq. (4). The choice of this parameter can be based on the Hansen's L-curve criterion which calculates the residual $\|A\alpha - b\|$ versus the norm of the solution $\|b\|$ for various

Table 1: ME, RE and RMSE with different time steps Δt and final time t_f and $\lambda = 10^{-11}$ for Example 1.

	$Errors$	$\Delta t = 1/3$	$\Delta t = 1/4$	$\Delta t = 1/8$	$\Delta t = 1/12$	$\Delta t = 1/20$
$t_f = 1$						
	ME	$9.2E-3$	$6.3E-3$	$7.0E-3$	$3.7E-3$	$3.0E-3$
	RE	$7.38E-2$	$4.96E-2$	$1.600E-1$	$1.041E-1$	$6.07E-2$
	$RMSE$	$5.774E-4$	$3.793E-4$	$4.726E-4$	$2.449E-4$	$2.047E-4$
$t_f = 2$						
	ME	$6.8E-3$	$5.1E-3$	$7.2E-3$	$5.7E-3$	$3.2E-3$
	RE	$7.67E-2$	$4.98E-2$	$1.603E-1$	$1.057E-1$	$6.25E-2$
	$RMSE$	$4.309E-4$	$3.106E-4$	$4.861E-4$	$3.892E-4$	$2.15E-4$
$t_f = 3$						
	ME	$1.4E-4$	$6.553E-4$	$1.708E-4E-4$	$4.121E-4$	$4.031E-4$
	ME	$6.230E-2$	$4.810E-2$	$1.793E-4E-1$	$1.298E-1$	$7.900E-2$
	$RMSE$	$8.333E-5$	$3.877E-5$	$1.090E-5$	$2.716E-5$	$2.629E-5$

Table 2: ME, RE and RMSE with time steps $\Delta t = 0.1$ and final time $t_f = 3$ and different values of λ Example 1.

$Errors$	$\lambda = 10^{-10}$	$\lambda = 10^{-11}$	$\lambda = 10^{-12}$	$\lambda = 10^{-13}$	$\lambda = 10^{-14}$
ME	$3.758E-4$	$3.818E-4$	$2.907E-4$	$3.280E-4$	$3.520E-4$
RE	$1.652E-1$	$1.689E-1$	$1.559E-1$	$1.445E-1$	$1.232E-1$
$RMSE$	$2.478E-5$	$2.521E-5$	$1.867E-5$	$2.164E-5$	$2.331E-5$

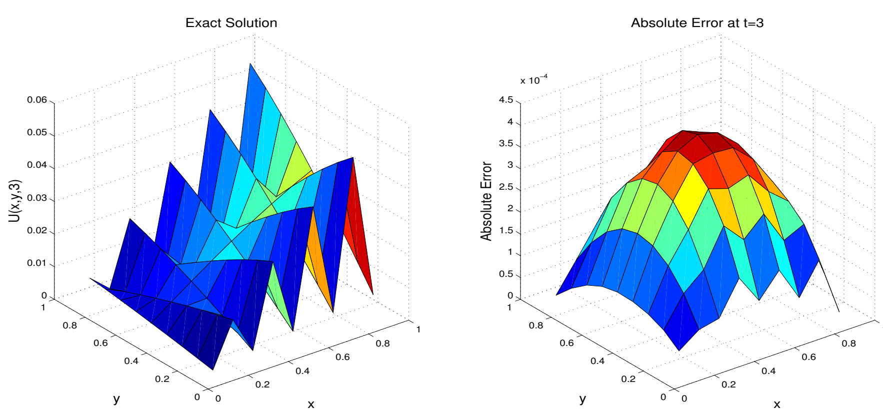

Figure 2: The numerical solution $\hat{u}$ and the absolute error at $t_f = 3$ for $N_i = 81$, $N_b = 40$, $\Delta t = 0.05$ and $\lambda = 10^{-11}$ for Example 1.

values of λ. In this work, we choose the regularization parameter λ by trial and error. In Table 2, the ME, RE and RMSE errors for different values of λ with time step $\Delta t = 0.1$ and final time $t_f = 3$ are presented to indicate the sensitivity of choosing the regularization parameter λ.

Example 2. Consider the following non-homogeneous two-dimensional problem

$$\frac{\partial u(\boldsymbol{x},t)}{\partial t} - \triangle u(\boldsymbol{x},t) - \nabla u(\boldsymbol{x},t) = f(\boldsymbol{x},t); \ t \in (0,t_f), \quad \mathbf{x} = (x,y),$$

where

$$f(\mathbf{x},t) = \frac{-2t(x^2+y^2)}{(1+t^2)^2} - \frac{2x+2y+4}{1+t^2}.$$

with the initial condition $u(\mathbf{x},0) = x^2+y^2$ for $(x,y) \in \bar{\Omega}$, and the boundary condition

$$u(\mathbf{x},t) = \frac{x^2+y^2}{1+t^2} \quad (x,y) \in \partial\Omega, \quad t > 0, \tag{14}$$

and the domain Ω is the same as that of Example 1. The analytical solution of the problem is given as

$$u(x,y,t) = \frac{x^2+y^2}{1+t^2}. \tag{15}$$

We have taken $N_i = 81, N_b = 40$ in our computations. In Table 2, the ME, RE and RMSE for numerical solution with different time step sizes are given. Moreover, the numerical solution $\hat{u}$ and the absolute difference between the numerical solution and the exact solution are shown in Fig. 3 for $\Delta t = 0.04$ at the final time $t_f = 3$.

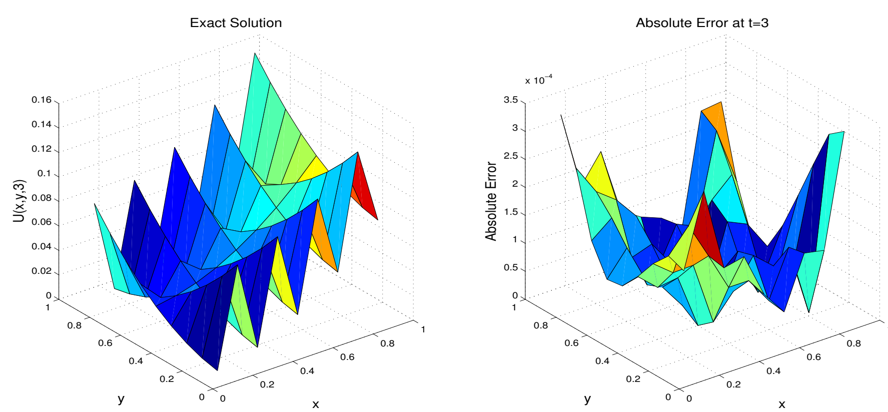

Figure 3: The numerical solution $\hat{u}$ and the absolute error at $t_f = 0.5$ for $\Delta t = 0.1$ for Example 2.

The different time increments indicate that smaller time increments give better results. Also, in Table 4, the ME, RE and RMSE errors for different values of λ with time step $\Delta t = 0.1$ and final time $t_f = 3$ are presented to indicate the sensitivity of choosing the regularization parameter λ.

Table 3: ME, RE and RMSE with different time steps Δt and final time t_f and $\lambda = 10^{-11}$ for Example 2.

		$\Delta t = 1/3$	$\Delta t = 1/4$	$\Delta t = 1/8$	$\Delta t = 1/15$	$\Delta t = 1/25$
$t_f = 1$						
	ME	$1.15E-3$	$6.400E-3$	$7.600E-3$	$5.500E-3$	$1.700E-3$
	RE	$1.403E-1$	$7.800E-3$	$1.120E-1$	$3.480E-2$	$1.260E-2$
	$RMSE$	$8.875E-4$	$5.314E-4$	$5.962E-4$	$3.869E-4$	$8.460E-5$
$t_f = 2$						
	ME	$4.700E-3$	$2.500E-3$	$3.00E-3$	$2.200E-3$	$6.717E-4$
	RE	$1.303E-3$	$1.800E-3$	$1.073E-1$	$3.600E-2$	$1.19E-2$
	$RMSE$	$3.627E-4$	$2.124E-4$	$2.365E-4$	$1.535E-4$	$3.348E-5$
$t_f = 3$						
	ME	$2.400E-3$	$1.200E-3$	$1.500E-3$	$1.100E-3$	$3.340E-4$
	RE	$1.213E-1$	$5.100E-3$	$9.960E-2$	$3.930E-2$	$9.700E-3$
	$RMSE$	$1.839E-4$	$1.046E-4$	$1.143E-4$	$7.424E-4$	$1.600E-5$

Table 4: ME, RE and RMSE with time steps $\Delta t = 0.1$ and final time $t_f = 3$ and different λ Example 2.

$Errors$	$\lambda = 10^{-10}$	$\lambda = 10^{-11}$	$\lambda = 10^{-12}$	$\lambda = 10^{-13}$	$\lambda = 10^{-14}$
ME	$1.3E-3$	$8.999E-4$	$4.948E-4$	$1.2E-3$	$1.2E-3$
RE	$1.267E-1$	$9.14E-2$	$1.838E-2$	$8.15E-2$	$6.3E-2$
$RMSE$	$1.104E-4$	$7.934E-5$	$2.561E-5$	$7.729E-5$	$6.962E-5$

6 Conclusions

In this paper, we used a numerical method with a time-dependent heat source for solving the non-homogeneous time-dependent convection-diffusion equations. This scheme is based on the fundamental solution of the diffusion equation with boundary meshfree property. Moreover, due to the meshfree nature of the proposed method, it is easy to implement with computational efficiency and it is applicable to higher dimensional problems with irregular geometry. The solutions are obtained by time-marching at all time levels by choosing appropriate source points and field points at the time levels. Also, Tikhonov regularization method was used to overcome the dilemma of conditioning in the linear system of equations. Finally, the stability and accuracy of the solution was confirmed by obtained numerical results.

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