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Research Article

CUBIC B-SPLINE LEAST SQUARES METHOD FOR THE NUMERICAL SOLUTION OF ADVECTION-DIFFUSION EQUATION

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Abstract. Least squares algorithm is set up for getting solution of the time dependent one dimensional advection-diffusion equation (ADE). The cubic B-spline least squares method is coupled with the Crank-Nicolson scheme to produce the numerical method which is used to integrate the ADE fully. Two test problems are studied to illustrate the efficiency of the proposed method.

Keywords: Advection-diffusion equation; least squares method; cubic B-spline.

AMS Subject Classification: 35C07; 35Q99; 65D07; 65M70; 76B25.

1. Introduction

Our environment has been contaminated everyday from industrial sources and plants. The study of contaminant transport require the knowledge of basic sciences such as mathematics and physics. Transportation of contaminants and contamination rate can be determined by way of mathematical modeling. ADE has served to model the transport of contamination in media. Combination of $\frac{\partial U}{\partial t}$, advection $\frac{\partial U}{\partial x}$ and diffusion $\frac{\partial^2 U}{\partial x^2}$ terms constitute the ADE:

$$\frac{\partial u(x,t)}{\partial t}+\epsilon\frac{\partial u(x,t)}{\partial x}-\gamma\frac{\partial^2 u(x,t)}{\partial x^2}=0, \quad x\in[a,b], \quad t\geq 0, \tag{1.1}$$

where ϵ and γ are parameters, t and x are time and space coordinates respectively. The initial condition (IC) is given as

$$u(x,0)=f(x). \tag{1.2}$$

Dirichlet boundary conditions (BCs) are

$$u(a,t)=0, \quad u(b,t)=0. \tag{1.3}$$

ADE describes contaminant transportation $u(x,t)$ in a moving fluid with a constant speed ϵ and diffusion coefficient γ in x direction at time t. Finding solutions of the ADE is a long standing problem. The equation includes behaviors of both advection and diffusion processes

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depending upon value of ϵ (advection coefficient) and γ (diffusion coefficient). Many numerical methods have been constructed to display the interaction between advective and diffusive processes. When the equation becomes advection dominated, numerical methods may exhibit some combination of spurious oscillations and excessive numerical diffusion. Progress is going on to overcome such difficulties effectively. Intrinsic numerical methods must be built up to avoid undesirable solutions.

The least squares technique is not much common to solve partial differential equations due to application difficulties as much as the finite element method and finite difference method. But there exists least squares studies on solving partial differential equations. ADE are also handled by means of the least squares method. A space time least squares finite element scheme is constructed for advection-diffusion equation [1]. A p-version based space-time least squares finite element method is applied to solve the unsteady convection-diffusion equation [3]. A computational scheme based on weighted residual least squares method using cubic B-splines is developed to solve ADE in the study [5]. The space time least squares formulation using the linear and quadratic B-spline basis functions have been presented for solving the ADE in the studies [2, 4].

In this paper, time derivative and spatial derivatives of ADE are discretized by help of the Crank-Nicolson method and the cubic B-spline least squares method respectively. This new algorithm is described in section 2. Accuracy of presented method is demonstrated by studying two test problems in the section of numerical simulations.

2. Cubic B-spline Least Squares Method

Consider equally distributed mesh points $a = x_0 < x_1 < x_2 < ... < x_N = b$ with $h = (b - a)/N$ and $x_m = x_0 + mh$ together with fictitious points x_{-3}, x_{-2}, x_{-1}, x_{N+1}, x_{N+2}, x_{N+3} outside the domain $[a, b]$. The cubic B-spline basis functions $B_m(x) \in C^2[a, b]$ at the grid points are defined as

$$B_m(x) = \frac{1}{h^3}\begin{cases} (x-x_{m-2})^3, & \text{if } x \in [x_{m-2}, x_{m-1}] \\ h^3 + 3h^2(x-x_{m-1}) + 3h(x-x_{m-1})^2 - 3(x-x_{m-1})^3, & \text{if } x \in [x_{m-1}, x_m] \\ h^3 + 3h^2(x_{m-1}-x) + 3h(x_{m-1}-x)^2 - 3(x_{m-1}-x)^3, & \text{if } x \in [x_m, x_{m+1}] \\ (x_{m+2}-x)^3, & \text{if } x \in [x_{m+1}, x_{m+2}] \\ 0, & \text{otherwise.} \end{cases} \tag{2.1}$$

Approximate solution $U(x, t)$ is given by an expansion of the cubic B-splines as:

$$u(x,t) \approx U(x,t) = \sum_{m=-1}^{N+1} B_m(x)\,\phi_m(t), \tag{2.2}$$

$\phi_m(t)$ are time dependent parameters determined by the least squares method. Approximation over subelements $[x_m, x_{m+1}]$, $\quad m = 0, \dots, N-1$ has following form:

$$U^e = B_{m-2}(x)\,\phi_{m-2}(t) + B_{m-1}(x)\,\phi_{m-1}(t) + B_m(x)\,\phi_m(t) + B_{m+1}(x)\,\phi_{m+1}(t) \tag{2.3}$$

where quantities $\phi_j(t), j = m-2, m-1, m, m+1$ are element parameters and $B_j(x), j = m-2, m-1, m, m+1$ are element shape functions. Introducing the change of variable

$$\xi = (x - x_m)/\Delta x, 0 \le \xi \le 1 \tag{2.4}$$

yields B-spline shape functions:

$$\begin{aligned} &B_{m-2}(\xi) = (1-\xi)^3, \\ &B_{m-1}(\xi) = 1 + 3(1-\xi) + 3(1-\xi)^2 - 3(1-\xi)^3, \\ &B_m(\xi) = 1 + 3\xi + 3\xi^2 - 3\xi^3, \\ &B_{m+1}(\xi) = \xi^3. \end{aligned}$$

The approximate solution and its first two derivatives at the grid points can be computed from the cubic B-spline functions as:

$$
\begin{aligned}
U_m &= U(x_m,t) = \phi_{m-1} + 4\phi_m + \phi_{m+1},\\
U'_m &= U'(x_m,t) = \tfrac{1}{h}(-3\phi_{m-1} + 3\phi_{m+1}),\\
U''_m &= U''(x_m,t) = \tfrac{6}{h^2}(\phi_{m-1} - 2\phi_m + \phi_{m+1}).
\end{aligned} \tag{2.5}
$$

Discretization of the ADE in time using the Crank-Nicolson method yields:

$$
2(U^{n+1} - U^n) + \beta(U_\xi^{n+1} + U_\xi^n) - \theta(U_{\xi\xi}^{n+1} + U_{\xi\xi}^n) = 0
$$

where $\beta = \epsilon\dfrac{\Delta t}{\Delta x}, \theta = \gamma\dfrac{\Delta t}{\Delta x^2}$.

Applying least squares technique to Eq. (1.1) and transformation defined above (2.4) yields the integral equation:

$$
\int_0^1 [2(U^{n+1} - U^n) + \beta(U_\xi^{n+1} + U_\xi^n) - \theta(U_{\xi\xi}^{n+1} + U_{\xi\xi}^n)]^2 d\xi = 0. \tag{2.6}
$$

Substitution of the approximation (2.2) and its derivatives in Eq. (2.6) leads to

$$
\sum_{j=m-2}^{m+1} \int_0^1 [2\left(Q_j(\xi)\phi_j^{n+1} - Q_j(\xi)\phi_j^n\right) + \beta(Q'_j(\xi)\phi_j^{n+1} + Q'_j(\xi)\phi_j^n) - \theta(Q''_j(\xi)\phi_j^{n+1} + Q''_j(\xi)\phi_j^n))]^2 d\xi = 0. \tag{2.7}
$$

Taking partial derivatives of the Eq. (2.7) with respect to time variable ϕ_i^{n+1}, and integration lead to a system of equations:

$$
\begin{aligned}
&[4A^e + 2\beta((B^e)^T + B^e) - 2\theta((C^e)^T + C^e) + \beta^2 D^e - \beta\theta((E^e)^T + E^e) + \theta^2 F^e](\phi^e)^{n+1}\\
&= [4A^e + 2\beta((B^e)^T + B^e) - 2\theta((C^e)^T - C^e) - \beta^2 D^e + \beta\theta((E^e)^T + E^e+) - \theta^2 F^e](\phi^e)^n
\end{aligned} \tag{2.8}
$$

where $\phi^e = (\phi_{m-2}, \phi_{m-1}, \phi_m, \phi_{m+1})$ are element parameters and the element matrices are given by the following integrals:

$$
\begin{aligned}
A^e &= \int_0^1 Q_i Q_j d\xi, \quad B^e = \int_0^1 Q_i Q'_j d\xi, \quad C^e = \int_0^1 Q_i Q''_j d\xi,\\
D^e &= \int_0^1 Q'_i Q'_j d\xi, \quad E^e = \int_0^1 Q'_i Q''_j d\xi, \quad F^e = \int_0^1 Q''_i Q''_j d\xi
\end{aligned}
$$

where i, j take only the values $m-2, m-1, m, m+1$ for the element $[x_m, x_{m+1}]$.

Assembling all contributions from all elements yields the global system of equations:

$$
\begin{aligned}
&[4A + 2\beta(B^T + B) - 2\theta(C^T + C) + \beta^2 D - \beta\theta(E^T + E) + \theta^2 F]\phi^{n+1}\\
&= [4A + 2\beta(B^T - B) - 2\theta(C^T - C) - \beta^2 D + \beta\theta(E^T + E) - \theta^2 F^e]\phi^n,
\end{aligned} \tag{2.9}
$$

where a vector of all nodal parameters is $\phi = (\phi_{-1}, \phi_0, \ldots, \phi_N, \phi_{N+1})^T$. A, B, B^T, C, C^T, D, E, E^T and F are derived from the element matrices A^e, B^e, $(B^e)^T$, C^e, $(C^e)^T$, D^e, E^e, $(E^e)^T$ and F^e, respectively.

After finding the parameters ϕ^{n+1}, approximate solution over the elements can be found with expression (2.3). Solution and its derivatives at the grid points can be directly computed with expression (2.5). Initial parameters ϕ_m^0 must be calculated using BCs and IC given in Eqs. (1.2)-(1.3) to give the algebraic equations below:

$$
\begin{aligned}
U(x_0,0) &= \phi_{-1}^0 + 4\phi_0^0 + \phi_1^0 = 0,\\
U(x_m,0) &= \phi_{m-1}^0 + 4\phi_m^0 + \phi_{m+1}^0 = f(x), \quad m = 0,\ldots,N,\\
U(x_N,0) &= \phi_{N-1}^0 + 4\phi_N^0 + \phi_{N+1}^0 = 0,
\end{aligned} \tag{2.10}
$$

from which we obtain initial parameters and use to start recursive formula to calculate approximate solution at required times t^n.

TABLE 1. Error norm for the Problem 1 at $t = 9600$

$h = \Delta t$	LSM	[6]	[7]	[8]	[6]
50	1.89×10^{-1}	1.90×10^{-1}	1.98×10^{-1}	3.73×10^{-1}	1.17×10^{-4}
10	7.50×10^{-3}	7.50×10^{-3}	7.51×10^{-3}	–	1.88×10^{-7}
5	1.87×10^{-3}	1.88×10^{-3}	–	–	1.17×10^{-8}
2	3.00×10^{-4}	3.00×10^{-4}	–	–	3.01×10^{-10}
1	7.50×10^{-5}	7.50×10^{-5}	7.50×10^{-5}	3.79×10^{-1}	2.21×10^{-11}

3. Numerical Simulations

L_∞ error norm

$$\|u - U\|_\infty = \max_j |u_j - U_j| \tag{3.1}$$

will be computed to measure the accuracy of the numerical scheme. Both pure advection and diffusion dominated problems are worked out to demonstrate the efficiency of the method.

3.1. **Problem 1.** Analytical solution of the pure advection problem, when $\gamma = 0$, is given by

$$u(x,t) = 10\exp(-\frac{(x - x_0 - \epsilon t)^2}{2\rho^2}). \tag{3.2}$$

Boundary conditions $u(0,t) = u(9000,t) = 0$ and initial condition $u(x,0)$ are used together with parameters $\rho = 264$m and $x_0 = 2000$. Run is carried out in spatial domain $[0, 900]$ until time $t = 9600$. L_∞ error norm of the presented method is tabulated together with some previous results in Table 1. When Crank-Nicolson approach is employed for the time discretization, all methods have produced the same accuracy seen in Table 1. Numerical solution at some times and its absolute error variation at time $t = 9600$ are graphed in Figure 1 (a)-(b) for space/time combination $h = \Delta t = 10$ respectively. Initial profile with constant height 10 advances to the right along x-axis.

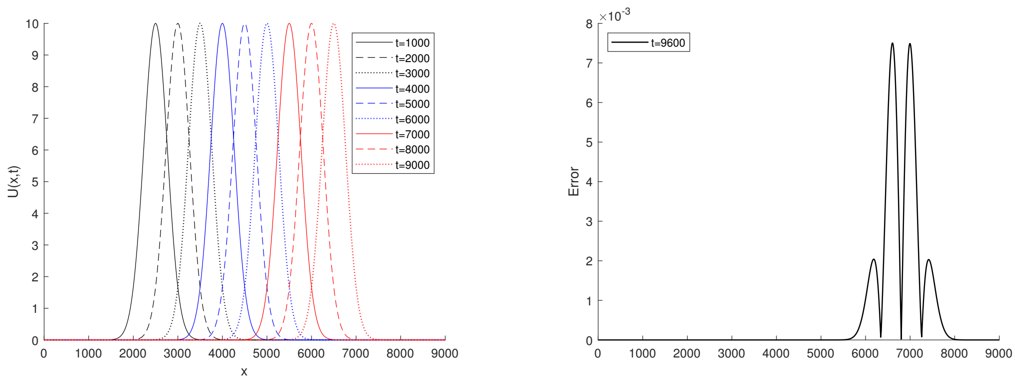

FIGURE 1. Numerical solutions at different times (left) and absolute error at $t = 9600$ (right)

3.2. **Problem 2.** The diffusion dominated solution of ADE is

$$u(x,t) = \frac{1}{\sqrt{4t+1}}\exp(-\frac{(x - x_0 - \epsilon t)^2}{\gamma(4t+1)}). \tag{3.3}$$

This solution represents fading of initial bell shaped profile. Initial wave profile of magnitude $\frac{1}{\sqrt{4t+1}}$ is centered at x_0 in the problem domain $[a, b]$ and propagates with decreasing magnitude. Program is run up to terminating time $t = 5$ with the velocity coefficient $\epsilon = 0.8$ m/s, the diffusion coefficient $\gamma = 0.005\ m^2/s$, boundary conditions $u(0,t) = u(9,t) = 0$ in $0 \le x \le 9$.

TABLE 2. Error norm for the Problem 2 at $t = 5$

$h = \Delta t$	LSM	[6]
0.1	5.23×10^{-2}	5.36×10^{-2}
0.05	1.24×10^{-2}	1.41×10^{-2}
0.02	1.03×10^{-3}	2.17×10^{-3}
0.01	1.40×10^{-3}	5.38×10^{-4}
0.005	1.78×10^{-3}	1.34×10^{-4}

Numerical results are written in Table 2 for various time-step increments. Numerical solutions at some times are visualized in Fig. 2 and absolute error at $t = 5$ are depicted for $h = \Delta t = 0.005$.

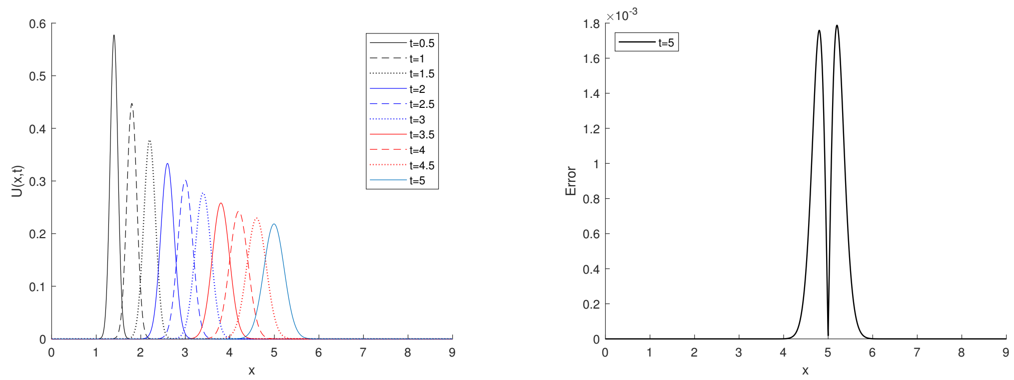

FIGURE 2. Numerical solutions at different times (left) and absolute error at $t = 5$ (right)

4. CONCLUSION

An numerical method is proposed for solving the ADE. The least squares approach turns into the Galerkin method in which trial functions are made up of the combination of the cubic B-splines. Thus, ADE is discretized by the suggested least squares method in spatial space and the Crank-Nicolson scheme in time to obtain a system of algebraic equations. The pure advection and the diffusion dominated problems are studied to show the achievement of the proposed scheme. The presented algorithm provides the same accuracy with results of the cubic B-spline Galerkin method and extended B-spline collocation method when the Crank-Nicolson technique is employed for time discretization of the ADE. If the high order time discretization is applied, the accuracy of the suggested method can also be increased. This case is shown in the study of M. Z. Gorgulu and D. Irk. Fourth order time discretization together with the cubic Galerkin method provides very accurate results seen in Table 1 of the their study [6]. Thus the suggested algorithm can be used as an alternative method for solving partial differential equations reliably.

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