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Higher Order Accurate Numerical Solution of Advection Diffusion Equation

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Abstract

In this study, the advection diffusion equation (ADE) will be solved numerically using the quintic B-spline Galerkin finite-element method, based on second and fourth order single step methods for time integration. Two test problems are studied and accuracy of the numerical results are measured by the computing the order of convergence and error norm L_∞ for the proposed methods. The numerical results of this study demonstrate that the proposed two algorithms especially the fourth order single step method are a remarkably successful numerical technique for solving the advection diffusion equation.

Keywords: *Advection diffusion equation; Galerkin method; quintic B-spline; Taylor series.*
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1. Introduction

The ADE (sometimes called the convection-diffusion equation) is the basis of many physical and chemical phenomena, and it is a one dimensional parabolic partial differential equation which illustrates advection and diffusion of quantities such as mass, energy, heat, vorticity etc.

Various numerical techniques have been developed and compared for solving the one dimensional ADE with constant coefficient so far. Dehghan [1] have developed the two-level finite difference approximations for solving the one dimensional ADE with constant coefficients. Up to tenth order finite difference schemes have been proposed to obtain numerical solution of the ADE in the study [2]. Least squares linear and quadratic B-spline finite element methods have been constructed in the study Dağ et.al [3]. In the study [4], cubic B-spline collocation and quadratic B-spline Galerkin finite elements methods have been used for the space discretization and Taylor series expansion has been used for the related time discretization for the numerical solution of the equation. Numerical solution of the ADE has been investigated using extended cubic B-spline finite element method in the study [5]. In the study [6], the quartic and quintic B-spline functions have been proposed to develop differential quadrature method to solve ADE, numerically.

This study presents a new time discretization numerical method for the advection-diffusion equation. The main idea of using this method is to obtain high-order approximate solution for ADE by using Taylor series expansion. The structure of the study is as follows. In the next section, after the time discretization of the advection-diffusion equation is performed by using higher accurate finite difference method, a finite element space discretization are used to obtain a system of algebraic equation. In the numerical experiment section, proposed methods are tested for the two test problems and finally, a summary of main findings of the work is presented in the last section.

We consider the following one dimensional ADE

$$u_t + \alpha u_x - \mu u_{xx} = 0,\ a \le x \le b \tag{1.1}$$

with the boundary conditions

$$\begin{matrix} u(a,t) = u(b,t) = 0 \\ u_x(a,t) = u_x(b,t) = 0 \end{matrix} \quad ,t \in [0,T] \tag{1.2}$$

and initial condition

$$u(x,0) = f(x),\ a \le x \le b \tag{1.3}$$

in a restricted solution domain over an space/time interval $[a,b] \times [0,T]$. In the one dimensional linear ADE, α is the steady uniform fluid velocity, μ is the constant diffusion coefficient and $u = u(x,t)$ is a function of two independent variables t and x, which generally denote time and space, respectively.

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2. Application of the Method

For computational work, the space-time plane is discretized by grids with the time step Δt and space step h. The exact solution of the unknown function at the grid points is denoted by

$$u(x_m,t_n) = u_m^n,\ m = 0,1,\ldots,N; \quad n = 0,1,2,\ldots$$

where $x_m = a+mh$, $t_n = n\Delta t$ and the notation U_m^n is used to represent the numerical value of u_m^n.

2.1. Time Discretization

Using the ADE of the form

$$u_t = \mu u_{xx} - \alpha u_x \tag{2.1}$$

and the following one-step method

$$u^{n+1} = u^n + \theta_1 u_t^{n+1} + \theta_2 u_t^n + \theta_3 u_{tt}^{n+1} + \theta_4^n u_{tt}^n, \tag{2.2}$$

we have the time discretization of the Eq. (2.1). If we take $\theta_1 = \theta_2 = \Delta t/2$, $\theta_3 = \theta_4 = 0$ in (2.2), the method is of order 2 (M1) known as Crank-Nicolson method (CN method) and then if we take $\theta_1 = \theta_2 = \dfrac{\Delta t}{2}$, $\theta_3 = -\dfrac{(\Delta t)^2}{12}$, $\theta_4 = \dfrac{(\Delta t)^2}{12}$, the method is of order 4 (M2), where Δt is time step. Using the (2.2) for the time discretization of the equation (2.1), we obtain

$$u^{n+1} - \theta_1 \left(\mu u_{xx} - \alpha u_x\right)^{n+1} - \theta_3 \left(\mu^2 u_{xxxx} - 2\alpha\mu u_{xxx} + \alpha^2 u_{xx}\right)^{n+1} = u^n + \theta_2 \left(\mu u_{xx} - \alpha u_x\right)^n + \theta_4 \left(\mu^2 u_{xxxx} - 2\alpha\mu u_{xxx} + \alpha u_{xx}\right)^n. \tag{2.3}$$

2.2. Quintic B-spline Galerkin Method

The interval $[a,b]$ is divided into uniformly sized finite subelements of equal length h at the knots

$$a = x_0 < x_1 < \ldots < x_N = b \tag{2.4}$$

where $h = x_m - x_{m-1} = (b-a)/N$, $m = 1,\ldots,N$. On this partition, the quintic B-splines ϕ_m, $m = -2,\ldots,N+2$, have the following form [6, 7, 8, 9, 10]:

$$\phi_m(x) = \frac{1}{h^5}\begin{cases}
(x-x_{m-3})^5, & [x_{m-3},x_{m-2}]\\
(x-x_{m-3})^5 - 6(x-x_{m-2})^5, & [x_{m-2},x_{m-1}]\\
(x-x_{m-3})^5 - 6(x-x_{m-2})^5 + 15(x-x_{m-1})^5, & [x_{m-1},x_m]\\
(x-x_{m-3})^5 - 6(x-x_{m-2})^5 + 15(x-x_{m-1})^5 - 20(x-x_m)^5, & [x_m,x_{m+1}]\\
(x-x_{m-3})^5 - 6(x-x_{m-2})^5 + 15(x-x_{m-1})^5 - 20(x-x_m)^5 + 15(x-x_{m+1})^5, & [x_{m+1},x_{m+2}]\\
(x-x_{m-3})^5 - 6(x-x_{m-2})^5 + 15(x-x_{m-1})^5 - 20(x-x_m)^5 + 15(x-x_{m+1})^5 - 6(x-x_{m+2})^5, & [x_{m+2},x_{m+3}]\\
0, & \text{otherwise}
\end{cases} \tag{2.5}$$

The set of quintic B-splines $\phi_m(x)$, $m = -2,\ldots,N+2$ forms a basis over the space interval $a \le x \le b$ [11]. Over the problem domain, the approximate solution $U(x,t)$ to the exact solution $u(x,t)$ can be written as a combination of the quintic B-splines

$$U(x,t) = \sum_{j=-2}^{N+2} \delta_j \phi_j \tag{2.6}$$

where δ_j are time dependent unknown parameters which will be determined from the Galerkin method and the boundary and initial conditions. Since the quintic B-spline functions (2.5) and its first four derivatives are continuous, trial solutions (2.6) have continuity up to fourth order. Using (2.5-2.6), the nodal values U and its first, second, third and fourth space derivatives at the knots x_m are obtained as

$$\begin{aligned}
U_m &= U(x_m) = \delta_{m+2} + 26\delta_{m+1} + 66\delta_m + 26\delta_{m-1} + \delta_{m-2},\\
U_m' &= U'(x_m) = \frac{5}{h}\left(\delta_{m+2} + 10\delta_{m+1} - 10\delta_{m-1} - \delta_{m-2}\right),\\
U_m'' &= U''(x_m) = \frac{20}{h^2}\left(\delta_{m+2} + 2\delta_{m+1} - 6\delta_m + 2\delta_{m-1} + \delta_{m-2}\right),\\
U_m''' &= U'''(x_m) = \frac{60}{h^3}\left(\delta_{m+2} - 2\delta_{m+1} + 2\delta_{m-1} - \delta_{m-2}\right),\\
U_m^{(4)} &= U^{(4)}(x_m) = \frac{120}{h^4}\left(\delta_{m+2} - 4\delta_{m+1} + 6\delta_m - 4\delta_{m-1} + \delta_{m-2}\right).
\end{aligned} \tag{2.7}$$

A typical finite interval $[x_m, x_{m+1}]$ is mapped to the interval $[0,h]$ by a local coordinate transformation defined by $\xi = x - x_m$. Therefore quintic B-spline shape functions in terms of ξ over the element $[0,h]$ can be given as

$$\begin{aligned}
\phi_{m-2}(\xi) &= 1-5\tfrac{\xi}{h}+10\left(\tfrac{\xi}{h}\right)^2-10\left(\tfrac{\xi}{h}\right)^3+5\left(\tfrac{\xi}{h}\right)^4-\left(\tfrac{\xi}{h}\right)^5,\\
\phi_{m-1}(\xi) &= 26-50\tfrac{\xi}{h}+20\left(\tfrac{\xi}{h}\right)^2+20\left(\tfrac{\xi}{h}\right)^3-20\left(\tfrac{\xi}{h}\right)^4+5\left(\tfrac{\xi}{h}\right)^5,\\
\phi_{m}(\xi) &= 66-60\left(\tfrac{\xi}{h}\right)^2+30\left(\tfrac{\xi}{h}\right)^4-10\left(\tfrac{\xi}{h}\right)^5,\\
\phi_{m+1}(\xi) &= 26+50\tfrac{\xi}{h}+20\left(\tfrac{\xi}{h}\right)^2-20\left(\tfrac{\xi}{h}\right)^3-20\left(\tfrac{\xi}{h}\right)^4+10\left(\tfrac{\xi}{h}\right)^5,\\
\phi_{m+2}(\xi) &= 1+5\tfrac{\xi}{h}+10\left(\tfrac{\xi}{h}\right)^2+10\left(\tfrac{\xi}{h}\right)^3+5\left(\tfrac{\xi}{h}\right)^4-5\left(\tfrac{\xi}{h}\right)^5,\\
\phi_{m+3}(\xi) &= \left(\tfrac{\xi}{h}\right)^5.
\end{aligned} \tag{2.8}$$

Combination of the element shape functions ϕ_i together with element time parameters δ_i, $i = m-2,\ldots,m+3$ gives an approximation for the typical element $[0,h]$

$$U^e = U(\xi,t) = \sum_{j=m-2}^{m+3} \delta_j(t)\phi_j(\xi). \tag{2.9}$$

Applying Galerkin method to Eq. (2.3) with weight function $W(x)$ leads to the equation:.

$$\begin{aligned}
&\int_a^b W(x)\left(u^{n+1}-\theta_1\left(\mu u_{xx}-\alpha u_x\right)^{n+1}-\theta_3\left(\mu^2 u_{xxxx}-2\alpha\mu u_{xxx}+\alpha^2 u_{xx}\right)^{n+1}\right)dx\\
&=\int_a^b W(x)\left(u^{n}+\theta_2\left(\mu u_{xx}-\alpha u_x\right)^{n}+\theta_4\left(\mu^2 u_{xxxx}-2\alpha\mu u_{xxx}+\alpha u_{xx}\right)^{n}\right)dx.
\end{aligned} \tag{2.10}$$

In the above Galerkin method formulation, weight functions $W(x)$ and exact solution are replaced with quintic B-splines shape functions (2.8) and approximation given by (2.9), respectively. Thus we obtain a fully discrete approximation is obtained over the element $[0,h]$ as

$$\begin{aligned}
&\sum_{j=m-2}^{m+3}\left(\int_0^h \phi_i\left(\phi_j-\theta_1\left(\mu\phi_j''-\alpha\phi_j'\right)-\theta_3\left(\mu^2\phi_j^{(4)}-2\alpha\mu\phi_j'''+\alpha^2\phi_j''\right)\right)d\xi\right)\delta_j^{n+1}\\
&-\sum_{j=m-2}^{m+3}\left(\int_0^h \phi_i\left(\phi_j+\theta_2\left(\mu\phi_j''-\alpha\phi_j'\right)+\theta_4\left(\mu^2\phi_j^{(4)}-2\alpha\mu\phi_j'''+\alpha^2\phi_j''\right)\right)d\xi\right)\delta_j^{n}
\end{aligned} \tag{2.11}$$

where i and j take only the values $m-2,\ldots,m+3$ and $m = 0,1,\ldots,N-1$ for the typical element $[0,h]$. (2.11) can be written in matrix form as

$$\left[\mathbf{A}^e-\theta_1\left(\mu\mathbf{C}^e-\alpha\mathbf{B}^e\right)-\theta_3\left(\mu^2\mathbf{E}^e-2\alpha\mu\mathbf{D}^e+\alpha^2\mathbf{C}^e\right)\right](\delta^e)^{n+1}-\left[\mathbf{A}^e+\theta_2\left(\mu\mathbf{C}^e-\alpha\mathbf{B}^e\right)+\theta_4\left(\mu^2\mathbf{E}^e-2\alpha\mu\mathbf{D}^e+\alpha^2\mathbf{C}^e\right)\right](\delta^e)^{n} \tag{2.12}$$

where the dimension of the element matrices $\mathbf{A}^e$, $\mathbf{B}^e$, $\mathbf{C}^e$, $\mathbf{D}^e$, $\mathbf{E}^e$ are 6×6, and the element matrices and element parameters are

$$A^e_{i,j}=\int_0^h \phi_i\phi_j d\xi, \qquad B^e_{i,j}=\int_0^h \phi_i\phi_j' d\xi, \qquad C^e_{i,j}=\int_0^h \phi_i\phi_j'' d\xi,$$

$$D^e_{i,j}=\int_0^h \phi_i\phi_j''' d\xi, \qquad E^e_{i,j}=\int_0^h \phi_i\phi_j^{(4)} d\xi, \qquad \delta^e=\left(\delta^n_{m-2},\ \ldots,\ \delta^n_{m+3}\right)^T.$$

Assembling contributions from all elements, (2.8) leads to the following linear system for the time evolution of δ:

$$\left[\mathbf{A}-\theta_1\left(\mu\mathbf{C}-\alpha\mathbf{B}\right)-\theta_3\left(\mu^2\mathbf{E}-2\alpha\mu\mathbf{D}+\alpha^2\mathbf{C}\right)\right]\delta^{n+1}=\left[\mathbf{A}+\theta_2\left(\mu\mathbf{C}-\alpha\mathbf{B}\right)+\theta_4\left(\mu^2\mathbf{E}-2\alpha\mu\mathbf{D}+\alpha^2\mathbf{C}\right)\right]\delta^{n}. \tag{2.13}$$

The linear system (2.13) consists of $N+5$ linear equations in $N+5$ unknowns $\left(\delta_{-2}^{n+1},\ldots,\delta_{N+2}^{n+1}\right)$. After the first and last equations are deleted in the system (2.13), imposition of the boundary conditions $U(a,x) = U(b,x) = 0$ at the both ends of the region yields to eliminate δ_{-2}^{n+1} and δ_{N+2}^{n+1} from the above system. Therefore the solution of the linear system with the dimensions $(N+3)\times(N+3)$ is obtained by way of Gauss elimination algorithms. After initial vector $\delta^0 = (\delta^0_{-2},\ldots,\delta^0_{N+2})$ is found with the help of the boundary and initial conditions, $\delta^{n+1}, (n = 0,1,\ldots)$ unknown vectors can be found repeatedly by solving the recurrence relation (2.13) using previous δ^n unknown vectors.

3. Numerical tests

For the test problems, accuracy of the proposed two algorithms is worked out by measuring error norm L_∞

$$L_\infty = \max_m |u_m - U_m|, \tag{3.1}$$

and the order of convergence is computed by the formula

$$\text{order}=\frac{\log\left|\dfrac{(L_\infty)_{h_i}}{(L_\infty)_{h_{i+1}}}\right|}{\log\left|\dfrac{h_i}{h_{i+1}}\right|}, \tag{3.2}$$

Table 1: Error norms L_∞ at time $t = 9600$ with $0 \le x \le 9000$

	M1		M2	
$h = \Delta t$	L_∞	Order	L_∞	Order
200	2.32		4.48×10^{-2}	
100	7.34×10^{-1}	1.66	1.75×10^{-3}	4.67
50	1.90×10^{-1}	1.95	1.16×10^{-4}	3.91
20	3.01×10^{-2}	2.01	3.00×10^{-6}	3.98
10	7.50×10^{-3}	2.00	1.88×10^{-7}	4.00
5	1.88×10^{-3}	2.00	1.17×10^{-8}	4.00
2	3.00×10^{-4}	2.00	3.06×10^{-10}	3.98
1	7.50×10^{-5}	2.00	3.92×10^{-11}	2.96

where $(L_\infty)_{h_i}$ is the error norm L_∞ for space step h_i.

Problem 1: Consider pure advection problem obtained by choosing $\mu = 0$. Then ADE has the exact solution

$$u(x,t) = 10\exp\left(-\frac{(x-\tilde{x}_0-\alpha t)^2}{2\rho^2}\right). \tag{3.3}$$

The numerical simulation is accomplished with flow velocity $\alpha = 0.5m/s$, initial peak location $\tilde{x}_0 = 2km$ and $\rho = 264$ by the terminating time $t = 9600s$. Therefore the initial condition $u(x,0)$ is propagated in a long channel without change in shape or size by the time $t = 9600s$ with flow velocity $\alpha = 0.5m/s$. So initial condition travels from the initial position to a distance of $4.8km$ and the peak value of the solution remain constant 10 for all time. After the program run up to time $t = 9600s$, initial solutions and waves are depicted in Fig. 1 for the M2 with $h = \Delta t = 1$. It can be seen from the figure that wave propagates without any change in its shape. Absolute error (difference between the exact and numerical solutions) distribution at $t = 9600s$ is also depicted in Fig.2. Since the maximum error occurs at about peak value of the wave at time $t = 9600s$, we can say that the effect of boundary conditions is negligible.

The error norms L_∞ and rate of convergence for the both proposed methods are listed in Table 1. According to the table, when time and space steps are reduced from 200 to 1, the error norms decrease for the both algorithms. It can also be seen that the rate of convergence is almost two for M1 and almost four for the M2. Therefore the proposed methods especially M2 are quite satisfactory.

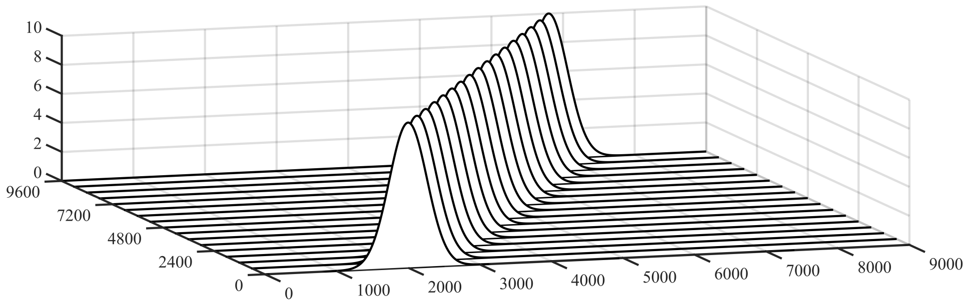

Figure 3.1: Wave profiles.

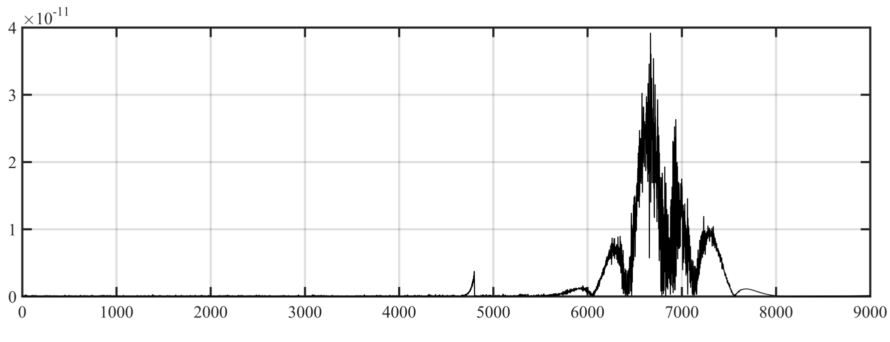

Figure 3.2: Absolute error for M2 with $h = \Delta t = 1$.

Problem 2: The exact solution of the ADE is

$$u(x,t) = \frac{1}{\sqrt{4t+1}}\exp\left(-\frac{(x-\tilde{x}_0-\alpha t)^2}{\mu\,(4t+1)}\right) \tag{3.4}$$

Table 2: Error norms L_∞ at time $t=5$ with $0 \le x \le 9$

	M1		M2	
$h=\Delta t$	L_∞	Order	L_∞	Order
0.05	1.41×10^{-2}	1.93	2.83×10^{-5}	
0.02	2.17×10^{-3}	2.04	7.32×10^{-7}	3.99
0.01	5.38×10^{-4}	2.01	4.60×10^{-8}	3.99
0.005	1.34×10^{-4}	2.00	2.87×10^{-9}	4.00
0.002	2.15×10^{-5}	2.00	7.36×10^{-11}	4.00
0.001	5.37×10^{-6}	2.00	5.56×10^{-12}	3.73

modelling fade out of an initial bell shaped concentration of height 1. This solution corresponds to a wave of magnitude $\dfrac{1}{\sqrt{4t+1}}$, initially centered on the position $\tilde{x}_0$ propagating towards the right across the interval $[a,b]$ over the up to the time T with a steady velocity α.
After the program run up to time $t=5$ with parameters $\alpha = 0.8\ m/s$, $\mu = 0.005\ m^2/s$ over the space interval $0 \le x \le 9$, error norms L_∞ and rate of convergence for both methods are listed in Table 2. It can be seen from the table that, when time and space steps are reduced from 0.05 to 0.001, the error norms decrease for the both algorithms. According to the error norms and rate of convergences in the table, the M2 generates better results than the M1 when the same time and space step sizes are used. It can also be seen that the rate of convergence is almost two for M1 and almost four for the M2 for this test problem.
Initial and numerical solutions for the M2 are drawn in Fig. 3 for visual view of the solution up to time $t=5$ over the space interval $[0,9]$ with $h=\Delta t=0.001$. Distribution of the absolute error at time is depicted for M2 with $h=\Delta t=0.001$ in Fig. 4. Maximum error is observed near the peak of the amplitude of the final wave.

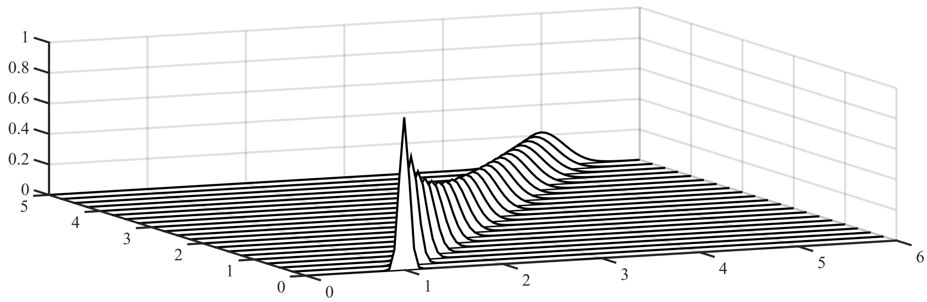

Figure 3.3: Fade out of initial pulse.

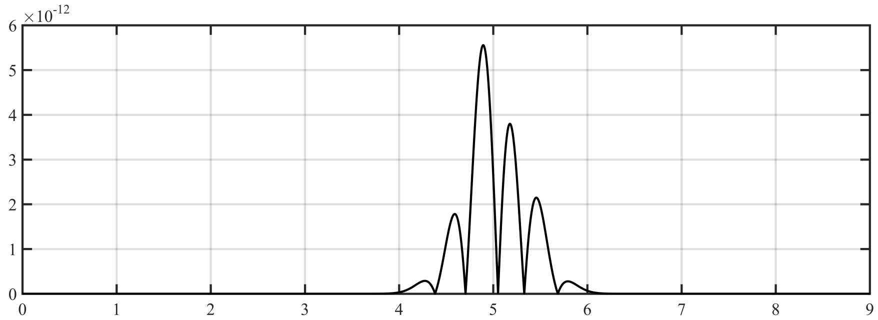

Figure 3.4: Absolute error for M2 with $h=\Delta t=0.001$.

4. Conclusion

The high-order Galerkin finite-element method based on Taylor series expansion for the time discretization and quintic B-spline functions for the space discretization was proposed to solve numerically the ADE. Two test problems were simulated well with the proposed two algorithms. Consequently, the numerical results of this study demonstrate that the proposed two algorithms especially the M2 are a remarkably successful numerical technique for solving the ADE. It can also be efficiently applied to similar physically important equations.

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