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A Stable Method for the Heat Equation Based on Simpson's Rule[1]

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Abstract

In this work we show how to use Simpson's rule and Simpson's 3/8 rule to obtain a numerical method for the approximation of the solution of the diffusion equation. In our numerical tests it appears that the method is stable independently of the step size in the discretization.

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1 Introduction

In this work we describe a numerical method based on Simpson's rule to approximate the solution of the difussion equation $\dfrac{\partial V}{\partial t} = \dfrac{\partial^2 V}{\partial x^2}$. As is well known, Simpson's rule has been used in numerical methods for the solution of initial value problems $y'(t) = f(t, y)$, $y(t_0) = y_0$, (see [2], [3], [4], [5]). All of these methods are conditionally stable, requiring small steps for stiff problems in order to yield accurate approximations. In [1] it was proposed an A-stable method for the numerical approximation of the initial value problem $y'(t) = f(t, y)$, $y(t_0) = y_0$.

In this paper we construct a method for the difussion equation based on the algorithm described in [1]. Our numerical tests show stability of the method independently of the step size in time in the discretization of the equation. The procedure is not a multistep method, and differs from most one-step methods in the sense that it simultaneously yields 3 approximations of the solution V at $t = t_0 + h$, $t_0 + 2h$, and $t_0 + 3h$ from the values of V at t_0.

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2 Discretization of the heat equation

Consider the heat equation

$$\frac{\partial V}{\partial t} = \frac{\partial^2 V}{\partial x^2}, \tag{1}$$

with boundary conditions

$$\begin{aligned} V(t_0, x) &= g(x) && (2)\\ V(t, 0) &= g_1(t) && (3)\\ V(t, 1) &= g_2(t). && (4)\\ & && (5) \end{aligned}$$

Adapting Simpson's 3/8 method (see [1]) to the diffusion equation (1) consists of three parts :

- Integrating both sides of (1) with respect to t from t_0 to t_2 and approximating the integral with Simpson's rule one obtains the approximation

$$V(t_2, x) - V(t_0, x) \approx \frac{h}{3}\left(\frac{\partial^2 V}{\partial x^2}(t_0, x) + 4\frac{\partial^2 V}{\partial x^2}(t_1, x) + \frac{\partial^2 V}{\partial x^2}(t_2, x)\right) \tag{6}$$

- Integrating both sides of (1) with respect to t from t_1 to t_3 and approximating the integral with Simpson's rule one obtains the approximation

$$V(t_3, x) - V(t_1, x) \approx \frac{h}{3}\left(\frac{\partial^2 V}{\partial x^2}(t_1, x) + 4\frac{\partial^2 V}{\partial x^2}(t_2, x) + \frac{\partial^2 V}{\partial x^2}(t_3, x)\right) \tag{7}$$

- Integrating both sides of (1) with respect to t from t_0 to t_3 and approximating the integral with Simpson's 3/8 rule one obtains the approximation

$$V(t_3, x) - V(t_0, x) \approx \frac{3h}{8}\left(\frac{\partial^2 V}{\partial x^2}(t_0, x) + 3\frac{\partial^2 V}{\partial x^2}(t_1, x) + 3\frac{\partial^2 V}{\partial x^2}(t_2, x) + \frac{\partial^2 V}{\partial x^2}(t_3, x)\right) \tag{8}$$

Let m be a positive integer, and let $\Delta x = 1/m$, $x_j = j\Delta x$ for $j = 0, 1, 2, ..., m$. We complement the discretization of (1) by making a finite difference approximation to second derivatives

$$\frac{\partial^2 V}{\partial x^2}(t_i, x_j) \approx \frac{V(t_i, x_{j+1}) - 2V(t_i, x_j) + V(t_i, x_{j-1})}{(\Delta x)^2}, \tag{9}$$

With the notation $V_{i,j} = V(t_i, x_j)$ and $c = \dfrac{h}{3(\Delta x)^2}$ we obtain from (6), (7), (8) and (9) the following approximations:

$$V_{2,j} - V_{0,j} \approx c(V_{0,j-1} - 2V_{0,j} + V_{0,j+1} + 4V_{1,j-1} - 8V_{1,j} + 4V_{1,j+1} + V_{2,j-1} - 2V_{2,j} + V_{2,j+1}) \tag{10}$$

$$V_{3,j} - V_{1,j} \approx c(V_{1,j-1} - 2V_{1,j} + V_{1,j+1} + 4V_{2,j-1} - 8V_{2,j} + 4V_{2,j+1} + V_{3,j-1} - 2V_{3,j} + V_{3,j+1}) \tag{11}$$

$$\begin{aligned} V_{3,j} - V_{0,j} &\approx \frac{3h}{8(\Delta x)^2}(V_{0,j-1} - 2V_{0,j} + V_{0,j+1} + 3V_{1,j-1} - 6V_{1,j} + 3V_{1,j+1} \\ &+ 3V_{2,j-1} - 6V_{2,j} + 3V_{2,j+1}) + V_{3,j-1} - 2V_{3,j} + V_{3,j+1}) \end{aligned} \tag{12}$$

From the last three approximations we set up a system of equation

$$U_{2,j} - U_{0,j} = c(U_{0,j-1} - 2U_{0,j} + U_{0,j+1} + 4U_{1,j-1} - U_{1,j} + U_{1,j+1} + U_{2,j-1} - 2U_{2,j} + U_{2,j+1}) \tag{13}$$

$$U_{3,j} - U_{1,j} = c(U_{1,j-1} - 2U_{1,j} + U_{1,j+1} + 4U_{2,j-1} - 8U_{2,j} + 4U_{2,j+1} + U_{3,j-1} - 2U_{3,j} + U_{3,j+1}) \tag{14}$$

$$\begin{aligned} U_{3,j} - U_{0,j} &= \frac{3h}{8(\Delta x)^2}(U_{0,j-1} - 2U_{0,j} + U_{0,j+1} + 3U_{1,j-1} - 6U_{1,j} + 3U_{1,j+1} \\ &+ 3U_{2,j-1} - 6U_{2,j} + 3U_{2,j+1}) + U_{3,j-1} - 2U_{3,j} + U_{3,j+1}) \end{aligned} \tag{15}$$

with $3(m-1)$ unknowns $U_{1,j}, U_{2,j}, U_{3,j}$ for $j = 1, 2, ..., m-1$, and where $U_{0,j} = V_{0,j}$ for $j = 0, 1, ..., m$, $U_{1,0} = V_{1,0}$, $U_{1,m} = V_{1,m}$, $U_{2,0} = V_{2,0}$, $U_{2,m} = V_{2,m}$, $U_{3,0} = V_{3,0}$, $U_{3,m} = V_{3,m}$.

By arranging the unknowns in the vector

$$w = (U_{1,1}\ U_{1,2}\ ...\ U_{1,m-1}\ U_{2,1}\ U_{2,2}\ ...\ U_{2,m-1}\ U_{3,1}\ U_{3,2}\ ...\ U_{3,m-1})^T,$$

we obtain a system of equations $Aw = b$, where the matrix $A \in \mathbb{R}^{3(m-1)\times 3(m-1)}$ is sparse and has a block structure of the form

$$A = \begin{pmatrix} A_1 & & A_2 & & A_3 & & \\ B_1 & & B_2 & & B_3 & & \\ & B_1 & & B_2 & & B_3 & \\ & & \cdot & & \cdot & & \cdot \\ & & & \cdot & & \cdot & \cdot \\ & & & B_1 & & B_2 & B_3 \\ & & & C_1 & & C_2 & C_3 \end{pmatrix}.$$

If $z_1 = \dfrac{h}{3(\Delta x)^2}$, $z_2 = \dfrac{3h}{8(\Delta x)^2}$, $k_1 = -2z_1 + 1$, $k_2 = -2z_2 - 1$, $k_3 = -2z_1 - 1$, the blocks are defined as follows:

$$B_1 = \begin{pmatrix} 4z_1 & -8z_1 & 4z_1 \\ z_1 & k_1 & z_1 \\ 3z_2 & -6z_2 & 3z_2 \end{pmatrix}, \; B_2 = \begin{pmatrix} z_1 & k_3 & z_1 \\ 4z_1 & -8z_1 & 4z_1 \\ 3z_2 & -6z_2 & 3z_2 \end{pmatrix}, \; B_3 = \begin{pmatrix} 0 & 0 & 0 \\ z_1 & k_3 & z_1 \\ z_2 & k_2 & z_2 \end{pmatrix},$$

$$A_1 = \begin{pmatrix} -8z_1 & 4z_1 & 0 \\ k_1 & z_1 & 0 \\ -6z_2 & 3z_2 & 0 \end{pmatrix}, \; A_2 = \begin{pmatrix} k_3 & z_1 & 0 \\ -8z_1 & 4z_1 & 0 \\ -6z_2 & 3z_2 & 0 \end{pmatrix}, \; A_3 = \begin{pmatrix} 0 & 0 & 0 \\ k_3 & z_1 & 0 \\ k_2 & z_2 & 0 \end{pmatrix},$$

$$C_1 = \begin{pmatrix} 4z_1 & -8z_1 \\ z_1 & k_1 \\ 3z_2 & -6z_2 \end{pmatrix}, \; C_2 = \begin{pmatrix} z_1 & k_3 \\ 4z_1 & -8z_1 \\ 3z_2 & -6z_2 \end{pmatrix}, \; C_3 = \begin{pmatrix} 0 & 0 \\ z_1 & k_3 \\ z_2 & k_2 \end{pmatrix}.$$

Denoting by $A_{[p..q,r..s]}$ the submatrix of A determined by rows i with $p \le i \le q$ and columns j with $r \le j \le s$, the blocks are distributed within the matrix A as follows:

$A_{[1..3,1..3]} = A_1$
$A_{[1..3,m..m+2]} = A_2$
$A_{[1..3,2m-1..2m+1]} = A_3$
$A_{[3m-5..3m-3,m-2..m-1]} = C_1$
$A_{[3m-5..3m-3,2m-3..2m-2]} = C_2$
$A_{[3m-5..3m-3,3m-4..3m-3]} = C_3$.

For integers r with $1 \le r \le p-2$ we have
$A_{[3r+1..3r+3,m-1+r..m+1+r]} = B_2$
$A_{[3r+1..3r+3,r..r+2]} = B_1$
$A_{[3r+1..3r+3,2m-2+r..2m+r]} = B_3$.

The right hand side b is defined as follows:

$b_1 = -z_1U_{0,0} - (-2z_1 + 1)U_{0,1} - z_1U_{0,2} - 4z_1U_{1,0} - z_1U_{2,0}$
$b_2 = -z_1U_{1,0} - 4z_1U_{2,0} - z_1U_{3,0}$
$b_3 = -z_2U_{0,0} - (-2z_2 + 1)U_{0,1} - z_2U_{0,2} - 3z_2U_{1,0} - 3z_2U_{2,0} - z_2U_{3,0}$
$b_{3m-5} = -z_1U_{0,m-2} - (-2z_1 + 1)U_{0,m-1} - z_1U_{0,m} - 4z_1U_{1,m} - z_1U_{2,m}$
$b_{3m-4} = -z_1U_{1,m} - 4z_1U_{2,m} - z_1U_{3,m}$
$b_{3m-3} = -z_2U_{0,m-2} - (-2z_2 + 1)U_{0,m-1} - z_2U_{0,m} - 3z_2U_{1,m} - 3z_2U_{2,m} - z_2U_{3,m}$

and for $q = 2, 3, ..., m-2$
$b_{3q-2} = -z_1U_{0,q-1} - (-2z_1 + 1)U_{0,q} - z_1U_{0,q+1}$
$b_{3q-1} = 0$
$b_{3q} = -z_2U_{0,q-1} - (-2z_2 + 1)U_{0,q} - z_2U_{0,q+1}$.

Once the vector of unknowns w is obtained by solving the system of equations $Aw = b$, we have the following approximations:
$V(t_1, x_j) \approx U_{1,j} = w_j$
$V(t_2, x_j) \approx U_{2,j} = w_{m+j-1}$
$V(t_3, x_j) \approx U_{3,j} = w_{2m+j-2}$.
for $j = 1, 2, ..., m-1$. To obtain approximations to $V(t_p, x_j)$ for $p = 4, 5, 6$ we repeat the above discretization taking now $U_{3,j}$, $j = 0, 1, ..., m$ as the initial values.

3 Numerical test

We tested the algorithm developed in the previous section using the following problem:

$$\frac{\partial V}{\partial t} = \frac{\partial^2 V}{\partial x^2}, \tag{16}$$

with boundary conditions

$$\begin{aligned} V(0,x) &= \sin(x), \text{ for } x \in [0,1] && (17)\\ V(t,0) &= 0 && (18)\\ V(t,1) &= e^{-t}\sin(1). && (19)\\ & && (20) \end{aligned}$$

The following table shows the relative errors of the approximation for two values of Δx, and several values of the time step h. Calculations were carried out at times $0 = t_0 < t_1 < ... < t_n = 1$, where $t_{i+1} = t_i + h$. The algorithm yields approximations of order 4 with respect to h.

h	Rel. Error with $\Delta x = 1/500$	Rel. Error with $\Delta x = 1/1000$
1/3	2.9×10^{-5}	2.9×10^{-5}
1/6	1.3×10^{-6}	1.3×10^{-6}
1/12	4.2×10^{-8}	5.3×10^{-8}
1/24	2.2×10^{-8}	3.6×10^{-9}

Table 1: Relative errors in the approximation of the solution of the heat equation. Approximations are done on a grid for $x \in [0,1]$ and $t \in [0,1]$.

As it can be seen on Table 1, for large values of the time step h compared to the size of $(\Delta x)^2$, the relative error of approximation remains small.

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