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Cover Page Footnote

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On the Consistency of Alternative Finite Difference Schemes for the Heat Equation

By *April Tran*

Abstract. While the well-researched Finite Difference Method (FDM) discretizes every independent variable into algebraic equations, Method of Lines discretizes all but one dimension, leaving an Ordinary Differential Equation (ODE) in the remaining dimension. That way, ODE's numerical methods can be applied to solve Partial Differential Equations (PDEs). In this project, Linear Multistep Methods and Method of Lines are used to numerically solve the heat equation. Specifically, the explicit Adams-Bashforth method and the implicit Backward Differentiation Formulas are implemented as Alternative Finite Difference Schemes. We also examine the consistency of these schemes.

1 Introduction

Finite Difference Methods are one of the most well-researched numerical techniques for solving Partial Differential Equations (PDEs). For these methods, finite difference is applied to approximate the derivatives. Both the time and the spatial domain are discretized, and the linear PDEs become systems of linear equations. Finite Difference Schemes (FDS) are specific Finite Difference Methods. For example, some widely used Finite Difference Schemes are Forward Time Centered Space FDS or Centered Time Centered Spaced FDS.

On the other hand, Method of Lines is another numerical technique for solving PDEs. Unlike Finite Difference Methods, Method of Lines discretizes all but one dimension, leaving an Ordinary Differential Equation (ODE) in the remaining dimension. In other words, Method of Lines transform PDEs into systems of ODEs, and ODEs numerical methods can then be used to solve PDEs.

One of the most used numerical techniques for solving ODEs is Linear Multistep Methods. Usually, a one-step numerical technique like the forward Euler's method solves an initial value problem by taking the starting point and a step forward in time. Meanwhile, Linear Multistep Methods use linear combinations of information from the previous steps to compute the next forward step.

In this paper, we propose the Alternative Finite Difference Schemes, which are achieved by combining Method of Lines and Linear Multistep Methods. Specifically,

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in section 2 we apply the Explicit Adams-Bashforth (AB) as well as the Backward Differentiation Formula (BDF) along with Method of Lines. In section 3, we examine the consistency of these schemes when applied to the heat equation.

2 Applying Method of Lines to the Heat Equation

Consider the heat equation $\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2}$ on a thin rod of length L with initial condition $u(x,0) = f(x)$ and boundary conditions $u(0,t)$ and $u(L,t)$. Divide the rod into N small pieces, each piece is Δx long and use centered finite difference to approximate $\frac{\partial^2 u}{\partial x^2}$ [2].

$$\frac{\partial u}{\partial t}(x_j,t) = \frac{\alpha}{\Delta x^2}\Big(U_{j+1}(t) - 2U_j(t) + U_{j-1}(t)\Big) \tag{1}$$

with $j = 1,2,\cdots,N-1$. The initial temperature distribution of the rod is given by $f(x)$ evaluated at $x_j \in [x_0, x_N]$. Indeed, $u(x_j,0) = U_j(0) = U_j^0 = f(x_j)$.

Note: The subscripts refer to the space step and the superscripts indicate time step. Notice U_j are function of t, so (1) really is an ODE of variable t with initial value given by $f(x)$. Method of Lines has transformed a PDE into a system of ODEs, and now we can use ODE numerical methods to solve this system. In this paper, Linear Multistep Methods are utilized. Specifically, the explicit Adams algorithm and Backward Differentiation Formula are applied.

2.1 Adams-Bashforth Methods

The Adams-Bashforth methods are among the most popular the explicit Linear Multistep Methods. The AB method are used to approximate solutions to the ODEs of the form $y' = g(t,y)$ with $y(t)$. The general formula for the Adams-Bashforth is [1, 5]:

$$y_n = y_{n-1} + h\sum_{j=1}^{k}\beta_j g_{n-j}$$

where h is the step size and

$$\beta_j = (-1)^{j-1}\sum_{i=j-1}^{k-1}\binom{i}{j-1}\gamma_i$$

$$\gamma_i = (-1)^i\int_0^1\binom{-s}{i}ds$$

Apply the $k-th$ order Adams-Bashforth to (1):

$$U_j^{m+1} = U_j^m + \Delta t \frac{\alpha}{\Delta x^2}\Big[\beta_1\Big(U_{j+1}^m - 2U_j^m + U_{j-1}^m\Big) + \beta_2\Big(U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}\Big) + \cdots + \beta_k\Big(U_{j+1}^{m-k+1} - 2U_j^{m-k+1} + U_{j-1}^{m-k+1}\Big)\Big] \tag{2.1.1}$$

Let $\alpha\frac{\Delta t}{\Delta x^2} = \sigma$, we have the finite difference schemes given by the explicit Adams method.

$$U_j^{m+1} = U_j^m + \sigma\Big[\beta_1\Big(U_{j+1}^m - 2U_j^m + U_{j-1}^m\Big) + \beta_2\Big(U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}\Big) + \cdots + \beta_k\Big(U_{j+1}^{m-k+1} - 2U_j^{m-k+1} + U_{j-1}^{m-k+1}\Big)\Big]$$

For example, we use Adams-Bashforth order 1, 2, and 3 to get the specific schemes. With the first order AB: $y_n = y_{n-1} + hg_{n-1}$, which is actually the Euler's method, we get:

$$U_j^{m+1} = U_j^m + \sigma\Big(U_{j+1}^m - 2U_j^m + U_{j-1}^m\Big)$$

This is in fact a well known and widely used finite difference scheme, forward time centered space. If we apply the second order AB: $y_n = y_{n-1} + h\left(\frac{3}{2}g_{n-1} - \frac{1}{2}g_{n-2}\right)$, we have:

$$U_j^{m+1} = U_j^m + \sigma\Big[\frac{3}{2}\Big(U_{j+1}^m - 2U_j^m + U_{j-1}\Big) - \frac{1}{2}\Big(U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}\Big)\Big]$$

This is the finite difference scheme given by second order Adams-Bashforth with the initial condition $U_j^0 = u(x_j, 0) = f(x_j)$ and boundary conditions $u_0^m = u(0, t_m)$ and $u_L^m = u(L, t_m)$. This can also be written in the matrix form. Let A and B be:

$$A = \begin{pmatrix} 1-3\sigma & \frac{3}{2}\sigma & 0 & 0 & \cdots & 0 \\ \frac{3}{2}\sigma & 1-3\sigma & \frac{3}{2}\sigma & 0 & \cdots & 0 \\ 0 & \frac{3}{2}\sigma & 1-3\sigma & \frac{3}{2}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{3}{2}\sigma & 1-3\sigma & \frac{3}{2}\sigma \\ 0 & 0 & \cdots & 0 & \frac{3}{2}\sigma & 1-3\sigma \end{pmatrix}$$

$$B = \begin{pmatrix} -\sigma & \frac{1}{2}\sigma & 0 & 0 & \cdots & 0 \\ \frac{1}{2}\sigma & -\sigma & \frac{1}{2}\sigma & 0 & \cdots & 0 \\ 0 & \frac{1}{2}\sigma & -\sigma & \frac{1}{2}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2}\sigma & -\sigma & \frac{1}{2}\sigma \\ 0 & 0 & \cdots & 0 & \frac{1}{2}\sigma & -\sigma \end{pmatrix}$$

$$\begin{bmatrix} U_1^{m+1} \\ U_2^{m+1} \\ . \\ . \\ . \\ U_{N-2}^{m+1} \\ U_{N-1}^{m+1} \end{bmatrix} = A \begin{bmatrix} U_1^{m} \\ U_2^{m} \\ . \\ . \\ . \\ U_{N-2}^{m} \\ U_{N-1}^{m} \end{bmatrix} + \frac{3}{2}\sigma \begin{bmatrix} U_0^{m} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_N^{m} \end{bmatrix} - B \begin{bmatrix} U_1^{m-1} \\ U_2^{m-1} \\ . \\ . \\ . \\ U_{N-2}^{m-1} \\ U_{N-1}^{m-1} \end{bmatrix} - \frac{1}{2}\sigma \begin{bmatrix} U_0^{m-1} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_N^{m-1} \end{bmatrix}$$

Notice this scheme and all the other schemes proposed in this paper are multistep schemes, which require multiple time steps. Usually, with initial value problems, only one initial time step is known. Multistep schemes, on the other hand, require more than one step to compute the next. For example, the scheme above requires both $u(x_j, t_m)$ and $u(x_j, t_{m-1})$, while only $u(x_j, t_{m-1})$ is provided as the initial condition. Therefore, in order to commence this multistep schemes, we have to begin with lower-ordered schemes, which in this case is the FTCS-FDS. The same goes with every multistep scheme mentioned in this paper.

If we apply the third order Adams-Bashforth:

$$y_n = y_{n-1} + h\Big(\frac{23}{12}g_{n-1} - \frac{16}{12}g_{n-2} + \frac{5}{12}g_{n-3}\Big)$$

We get:

$$\begin{aligned} U_j^{m+1} = U_j^m + \sigma\Big[&\frac{23}{12}\Big(U_{j+1}^m - 2U_j^m + U_{j-1}^m\Big) \\ &-\frac{16}{12}\Big(U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}\Big) \\ &+\frac{5}{12}\Big(U_{j+1}^{m-2} - 2U_j^{m-2} + U_{j-1}^{m-2}\Big)\Big] \end{aligned}$$

Let A, B and C be:

$$A = \begin{pmatrix} 1-\frac{23}{6}\sigma & \frac{23}{12}\sigma & 0 & 0 & \cdots & 0 \\ \frac{23}{12}\sigma & 1-\frac{23}{6}\sigma & \frac{23}{12}\sigma & 0 & \cdots & 0 \\ 0 & \frac{23}{12}\sigma & 1-\frac{23}{6}\sigma & \frac{23}{12}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{23}{12}\sigma & 1-\frac{23}{6}\sigma & \frac{23}{12}\sigma \\ 0 & 0 & \cdots & 0 & \frac{23}{12}\sigma & 1-\frac{23}{6}\sigma \end{pmatrix}$$

$$B = \begin{pmatrix} -\frac{16}{6}\sigma & \frac{16}{12}\sigma & 0 & 0 & \cdots & 0 \\ \frac{16}{12}\sigma & -\frac{16}{6}\sigma & \frac{16}{12}\sigma & 0 & \cdots & 0 \\ 0 & \frac{16}{12}\sigma & -\frac{16}{6}\sigma & \frac{16}{12}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{16}{12}\sigma & -\frac{16}{6}\sigma & \frac{16}{12}\sigma \\ 0 & 0 & \cdots & 0 & \frac{16}{12}\sigma & -\frac{16}{6}\sigma \end{pmatrix}$$

$$C = \begin{pmatrix} -\frac{5}{6}\sigma & \frac{5}{12}\sigma & 0 & 0 & \cdots & 0 \\ \frac{5}{12}\sigma & -\frac{5}{6}\sigma & \frac{5}{12}\sigma & 0 & \cdots & 0 \\ 0 & \frac{5}{12}\sigma & -\frac{5}{6}\sigma & \frac{5}{12}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{5}{12}\sigma & -\frac{5}{6}\sigma & \frac{5}{12}\sigma \\ 0 & 0 & \cdots & 0 & \frac{5}{12}\sigma & -\frac{5}{6}\sigma \end{pmatrix}$$

The matrix form is:

$$\begin{aligned} \begin{bmatrix} U_1^{m+1} \\ U_2^{m+1} \\ . \\ . \\ . \\ U_{N-2}^{m+1} \\ U_{N-1}^{m+1} \end{bmatrix} &= A \begin{bmatrix} U_1^{m} \\ U_2^{m} \\ . \\ . \\ . \\ U_{N-2}^{m} \\ U_{N-1}^{m} \end{bmatrix} + \frac{23}{12}\sigma \begin{bmatrix} U_0^{m} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_{N}^{m} \end{bmatrix} \\ &- B \begin{bmatrix} U_1^{m-1} \\ U_2^{m-1} \\ . \\ . \\ . \\ U_{N-2}^{m-1} \\ U_{N-1}^{m-1} \end{bmatrix} - \frac{16}{12}\sigma \begin{bmatrix} U_0^{m-1} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_{N}^{m-1} \end{bmatrix} \\ &+ C \begin{bmatrix} U_1^{m-2} \\ U_2^{m-2} \\ . \\ . \\ . \\ U_{N-2}^{m-2} \\ U_{N-1}^{m-2} \end{bmatrix} + \frac{5}{12}\sigma \begin{bmatrix} U_0^{m-2} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_{N}^{m-2} \end{bmatrix} \end{aligned}$$

This is the finite difference scheme given by the third order Adams-Bashforth.

2.2 Backward Differentiation Formula

Next, we examine an implicit numerical technique, Backward Differentiation Formula (BDF). Similar to Adam-Bashforth, Backward Differentiation Formula are also used to approximate solutions to ODEs of the form $y' = g(t, y)$ with $y(t)$. The general formula for BDF is [1, 3]:

$$\sum_{j=1}^{k} \frac{1}{j} \nabla^i y_n = h g_n$$

This method is usually written in a scaled form where the coefficient of y_n is 1. By scaling the formula, a constant $\tau = \frac{1}{\alpha_0}$ appears on the right hand side:

$$\sum_{j=0}^{k} \alpha_i \nabla^i y_{n-j} = \tau h g_n$$

In this paper, we use the scaled form of Backward Differential Formula:

$$y_n + \alpha_1 y_{n-1} + \alpha_2 y_{n-2} + \cdots + \alpha_k y_{n-k} = \tau h f_n$$

Note: Backward Differentiation Formula with more than 6 steps are unstable. In this paper, we only cover from the first order to the sixth order BDF.

Apply the $k-th$ order Backward Differentiation Formula to (1):

$$U_j^{m+1} + \alpha_1 U_j^m + \cdots + \alpha_k U_j^{m-k+1} = \Delta t \frac{\alpha}{\Delta x^2} \tau \left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1} \right) \tag{2.2.1}$$

Let $\Delta t \frac{\alpha}{\Delta x^2} = \sigma$, and we get:

$$U_j^{m+1} + \alpha_1 U_j^m + \cdots + \alpha_k U_j^{m-k+1} = \sigma\tau \left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1} \right)$$

We apply Backward Differentiation Formula order 1, 2 and 3 to get the specific schemes. For the first order BDF $y_n - y_{n-1} = h g_n$ with $\tau = 1$, which is the backward Euler's method, we get the backward time centered spaced finite difference scheme. Meanwhile, if we apply the second order BDF: $y_n - \frac{4}{3} y_{n-1} + \frac{1}{3} y_{n-2} = \frac{2}{3} h g_n$ with $\tau = \frac{2}{3}$, we get:

$$U_j^{m+1} - \frac{4}{3} U_j^m + \frac{1}{3} U_j^{m-1} = \frac{2}{3} \sigma \left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1} \right)$$

So

$$\frac{4}{3} U_j^m - \frac{1}{3} U_j^{m-1} = -\frac{2}{3} \sigma U_{j+1}^{m+1} + \left(1 + \frac{4}{3} \sigma \right) U_j^{m+1} - \frac{2}{3} \sigma U_{j-1}^{m+1}$$

This is finite difference scheme given by the second order Backward Differentiation Formula. Let A be:

$$A = \begin{pmatrix} 1+\frac{4}{3}\sigma & -\frac{2}{3}\sigma & 0 & 0 & \cdots & 0 \\ -\frac{2}{3}\sigma & 1+\frac{4}{3}\sigma & -\frac{2}{3}\sigma & 0 & \cdots & 0 \\ 0 & -\frac{2}{3}\sigma & 1+\frac{4}{3}\sigma & -\frac{2}{3}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & -\frac{2}{3}\sigma & 1+\frac{4}{3}\sigma & -\frac{2}{3}\sigma \\ 0 & 0 & \cdots & 0 & -\frac{2}{3}\sigma & 1+\frac{4}{3}\sigma \end{pmatrix}$$

The matrix form would be:

$$\frac{4}{3}\begin{bmatrix} U_1^m \\ U_2^m \\ . \\ . \\ . \\ U_{N-2}^m \\ U_{N-1}^m \end{bmatrix} - \frac{1}{3}\begin{bmatrix} U_1^{m-1} \\ U_2^{m-1} \\ . \\ . \\ . \\ U_{N-2}^{m-1} \\ U_{N-1}^{m-1} \end{bmatrix} = A\begin{bmatrix} U_1^{m+1} \\ U_2^{m+1} \\ . \\ . \\ . \\ U_{N-2}^{m+1} \\ U_{N-1}^{m+1} \end{bmatrix} - \frac{2}{3}\sigma\begin{bmatrix} U_0^{m+1} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_N^{m+1} \end{bmatrix}$$

So:

$$\begin{bmatrix} U_1^{m+1} \\ U_2^{m+1} \\ . \\ . \\ . \\ U_{N-2}^{m+1} \\ U_{N-1}^{m+1} \end{bmatrix} = A^{-1}\left(\frac{4}{3}\begin{bmatrix} U_1^m \\ U_2^m \\ . \\ . \\ . \\ U_{N-2}^m \\ U_{N-1}^m \end{bmatrix} - \frac{1}{3}\begin{bmatrix} U_1^{m-1} \\ U_2^{m-1} \\ . \\ . \\ . \\ U_{N-2}^{m-1} \\ U_{N-1}^{m-1} \end{bmatrix} + \frac{2}{3}\sigma\begin{bmatrix} U_0^{m+1} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_N^{m+1} \end{bmatrix}\right)$$

Note: The Thomas algorithm can be used to solve for this tridiagonal system of equations instead of computing A^{-1}.

With the third order BDF: $y_n - \frac{18}{11}y_{n-1} + \frac{9}{11}y_{n-2} - \frac{2}{11}y_{n-3} = \frac{6}{11}hg_n$ with $\tau = \frac{6}{11}$, we have:

$$U_j^{m+1} - \frac{18}{11}U_j^m + \frac{9}{11}U_j^{m-1} - \frac{2}{11}U_j^{m-2} = \frac{6}{11}\sigma\left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}\right)$$

Which leads to:

$$\frac{18}{11}U_j^m - \frac{9}{11}U_j^{m-1} + \frac{2}{11}U_j^{m-2} = -\frac{6}{11}\sigma U_{j+1}^{m+1} + \left(1 + \frac{12}{11}\sigma\right)U_j^{m+1} - \frac{6}{11}\sigma U_{j-1}^{m+1}$$

This is finite difference scheme given by the third order Backward Differentiation Formula. Next, we examine the matrix form of this scheme. Let B be

$$B = \begin{pmatrix} 1+\frac{12}{11}\sigma & -\frac{6}{11}\sigma & 0 & 0 & \cdots & 0 \\ -\frac{6}{11}\sigma & 1+\frac{12}{11}\sigma & -\frac{6}{11}\sigma & 0 & \cdots & 0 \\ 0 & -\frac{6}{11}\sigma & 1+\frac{12}{11}\sigma & -\frac{6}{11}\sigma & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & -\frac{6}{11}\sigma & 1+\frac{12}{11}\sigma & -\frac{6}{11}\sigma \\ 0 & 0 & \cdots & 0 & -\frac{6}{11}\sigma & 1+\frac{12}{11}\sigma \end{pmatrix}$$

So the matrix form is:

$$\begin{bmatrix} U_1^{m+1} \\ U_2^{m+1} \\ . \\ . \\ . \\ U_{N-2}^{m+1} \\ U_{N-1}^{m+1} \end{bmatrix} = B^{-1} \left(\frac{18}{11} \begin{bmatrix} U_1^{m} \\ U_2^{m} \\ . \\ . \\ . \\ U_{N-2}^{m} \\ U_{N-1}^{m} \end{bmatrix} - \frac{9}{11} \begin{bmatrix} U_1^{m-1} \\ U_2^{m-1} \\ . \\ . \\ . \\ U_{N-2}^{m-1} \\ U_{N-1}^{m-1} \end{bmatrix} + \frac{2}{11} \begin{bmatrix} U_1^{m-2} \\ U_2^{m-2} \\ . \\ . \\ . \\ U_{N-2}^{m-2} \\ U_{N-1}^{m-2} \end{bmatrix} + \frac{6}{11}\sigma \begin{bmatrix} U_0^{m+1} \\ 0 \\ . \\ . \\ . \\ 0 \\ U_N^{m+1} \end{bmatrix} \right)$$

Note: Again, The Thomas algorithm can also be used to solve for this tridiagonal system of equations.

3 Consistency of Alternative Finite Difference Schemes

Next, we discuss the consistency of the Alternative Finite Difference Schemes. A Finite Difference Scheme is considered to be consistent if by reducing the time and space step, the difference between the actual solution and the solution given by the scheme could approach 0. The consistency can be explored using the Taylor expansion.

Definition 3.1 (Consistency)**.** Given a partial differential equation $P_\phi = f$ and finite difference scheme, $P_{\Delta x,\Delta t,\phi} = f$, we say the finite difference scheme is consistent with the partial differential equation if for any smooth function $\phi(t,x)$

$$P_\phi - P_{\Delta x,\Delta t,\phi} \to 0 \text{ as } \Delta x, \Delta t \to 0$$

the convergence being point wise convergence at each grid point [8].

3.1 Adams-Bashforth

We examine the consistency of the alternative finite difference scheme given the explicit Adams method on the heat equation. Starting with the partial differential equation:

$$P_u = \partial_t u - \alpha \partial_x^2 u$$

And the schemes given by Adams-Bashforth (2.1.1):

$$\begin{aligned}P_{\Delta x,\Delta t,u} = \frac{U_j^{m+1}-U_j^m}{\Delta t} - \frac{\alpha}{\Delta x^2}\Big[&\beta_1\Big(U_{j+1}^m - 2U_j^m + U_{j-1}^m\Big)\\ &+\beta_2\Big(U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}\Big)\\ &+\cdots+\\ &+\beta_k\Big(U_{j+1}^{m-k+1} - 2U_j^{m-k+1} + U_{j-1}^{m-k+1}\Big)\Big]\end{aligned}$$

As we can see in these schemes for the heat equation, there are 2 distinct components: time t component and space x component. We begin with the time component:

$$\frac{U_j^{m+1}-U_j^m}{\Delta t}$$

by taking the Taylor expansion of U_j^{m+1} about U_j^m with respect to t:

$$U_j^{m+1} = U_j^m + \Delta t \partial_t U_j^m + \frac{1}{2}\Delta t^2 \partial_t^2 U_j^m + O(\Delta t^3)$$

Note: $\partial_t^i U$ denotes the i-th ordered partial derivative of u with respect to t. The time component would be:

$$\frac{U_j^{m+1}-U_j^m}{\Delta t} = \partial_t U_j^m + \frac{1}{2}\Delta t \partial_t^2 U_j^m + O(\Delta t^2)$$

Next, we analyze the space component of these schemes:

$$\begin{aligned}\frac{\alpha}{\Delta x^2}\Big[&\beta_1\Big(U_{j+1}^m - 2U_j^m + U_{j-1}^m\Big)\\ &+\beta_2\Big(U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}\Big)\\ &+\cdots+\\ &+\beta_k\Big(U_{j+1}^{m-k+1} - 2U_j^{m-k+1} + U_{j-1}^{m-k+1}\Big)\Big]\end{aligned}$$

The space component consists of k centered finite difference approximations evaluated at k previous time steps. These approximations are scaled by the coefficients β_k given by Adams-Bashforth. For each of these approximations, we take the Taylor expansion of both space step U_{j+1} and U_{j-1} about U_j with respect to x.
For example, with $k=1$, we have:

$$\begin{aligned}U_{j+1}^m = U_j^m + \Delta x \partial_x U_j^m + \frac{1}{2}\Delta x^2 \partial_x^2 U_j^m + \frac{1}{6}\Delta x^3 \partial_x^3 U_j^m\\ + \frac{1}{24}\Delta x^4 \partial_x^4 U_j^m + O(\Delta x^5)\end{aligned}$$

$$U_{j-1}^m = U_j^m - \Delta x \partial_x U_j^m + \frac{1}{2}\Delta x^2 \partial_x^2 U_j^m - \frac{1}{6}\Delta x^3 \partial_x^3 U_j^m + \frac{1}{24}\Delta x^4 \partial_x^4 U_j^m + O(\Delta x^5)$$

So at $k=1$, $\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2}$ would be:

$$\frac{U_{j+1}^m - 2U_j^m + U_{j-1}^m}{\Delta x^2} = \partial_x^2 U_j^m + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^m + O(\Delta x^3)$$

Similarly, at $k=2$, we take the Taylor expansion of U_{j+1}^{m-1} and U_{j-1}^{m-1} about U_j^{m-1}:

$$\frac{U_{j+1}^{m-1} - 2U_j^{m-1} + U_{j-1}^{m-1}}{\Delta x^2} = \partial_x^2 U_j^{m-1} + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^{m-1} + O(\Delta x^3)$$

The same goes with $k=3$ and so on. In general, we have:

$$\frac{U_{j+1}^{m-k+1} - 2U_j^{m-k+1} + U_{j-1}^{m-k+1}}{\Delta x^2} = \partial_x^2 U_j^{m-k+1} + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^{m-k+1} + O(\Delta x^3)$$

Now, truncation errors are:

$$\begin{aligned} P_{u(x_j,t_m)} - P_{\Delta x,\Delta x,u(x_j,t_m)} = &\left(\partial_t U_j^m - \alpha \partial_x^2 U_j^m\right) - \Bigg\{\left(\partial_t U_j^m + \frac{1}{2}\Delta t \partial_t^2 U_j^m + O(\Delta t^2)\right) \\ &-\alpha\Bigg[\beta_1\left(\partial_x^2 U_j^m + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^m + O(\Delta x^3)\right) \\ &+\beta_2\left(\partial_x^2 U_j^{m-1} + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^{m-1} + O(\Delta x^3)\right) \\ &+\cdots+ \\ &+\beta_k\left(\partial_x^2 U_j^{m-k+1} + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^{m-k+1} + O(\Delta x^3)\right)\Bigg]\Bigg\} \end{aligned}$$

As Δt and Δx approach 0, we are left with:

$$\begin{aligned} \lim_{\Delta x,\Delta t\to 0} P_{u(x_j,t_m)} - P_{\Delta x,\Delta x,u(x_j,t_m)} = &\left(\partial_t U_j^m - \alpha \partial_x^2 U_j^m\right) - \Big\{\partial_t U_j^m \\ &-\alpha\Big[\lim_{\Delta x,\Delta t\to 0}\left(\beta_1 \partial_x^2 U_j^m + \beta_2 \partial_x^2 U_j^{m-1} + \cdots + +\beta_k \partial_x^2 U_j^{m-k+1}\right)\Big]\Big\} \end{aligned}$$

From here, we can cancel $\partial_t U_j^m$. Not only that, as Δt goes to 0, t_{m-1} gets closer to t_m, t_{m-2} also gets closer to t_m and so on. Therefore, $\partial_x^2 U_j^{m-1}, \partial_x^2 U_j^{m-2}$, $\cdots, \partial_x^2 U_j^{m-k+1}$ all get closer to $\partial_x^2 U_j^m$. Moreover, for Adams-Bashforth methods, $\beta_1 + \beta_2 + \cdots + \beta_k = 1$. Consequently,:

$$\alpha\Big[\lim_{\Delta x,\Delta t\to 0}\left(\beta_1 \partial_x^2 U_j^m + \beta_2 \partial_x^2 U_j^{m-1} + \cdots + +\beta_k \partial_x^2 U_j^{m-k+1}\right)\Big] = \alpha \partial_x^2 U_j^m$$

Which means:

$$P_{u(x_j,t_m)} - P_{\Delta x,\Delta x,u(x_j,t_m)} = 0$$

as Δt approaches 0. Therefore, the finite difference schemes given by Adams-Bashforth method are consistent.

3.2 Backward Differentiation Formula

Again, we examine the consistency of the schemes given by the Backward Differentiation Formula on the heat equation. We start with the PDE:

$$P_u = \partial_t u - \alpha \partial_x^2 u$$

And the schemes:

$$P_{\Delta x,\Delta t,u} = \frac{U_j^{m+1} + \alpha_1 U_j^m + \cdots + \alpha_k U_j^{m-k+1}}{\Delta t} - \frac{\alpha}{\Delta x^2}\tau\left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}\right)$$

Which can also be written as:

$$P_{\Delta x,\Delta t,u} = \frac{\frac{1}{\tau}U_j^{m+1} + \frac{\alpha_1}{\tau}U_j^m + \cdots + \frac{\alpha_k}{\tau}U_j^{m-k+1}}{\Delta t} - \frac{\alpha}{\Delta x^2}\left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}\right)$$

Similar to the finite difference schemes given by Adams-Bashforth methods, these schemes also consist of 2 components: space and time. We begin with the space component:

$$\frac{\alpha}{\Delta x^2}\left(U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}\right)$$

We consider the Taylor expansion of U_{j+1}^{m+1} and U_{j-1}^{m+1} about U_j^{m+1} with respect to x:

$$\begin{aligned} U_{j+1}^{m+1} = U_j^{m+1} + \Delta x \partial_x U_j^{m+1} + \frac{1}{2}\Delta x^2 \partial_x^2 U_j^{m+1} + \frac{1}{6}\Delta x^3 \partial_x^3 U_j^{m+1} \\ + \frac{1}{24}\Delta x^4 \partial_x^4 U_j^{m+1} + O(\Delta x^5) \end{aligned}$$

$$\begin{aligned} U_{j-1}^{m+1} = U_j^{m+1} - \Delta x \partial_x U_j^{m+1} + \frac{1}{2}\Delta x^2 \partial_x^2 U_j^{m+1} - \frac{1}{6}\Delta x^3 \partial_x^3 U_j^{m+1} \\ + \frac{1}{24}\Delta x^4 \partial_x^4 U_j^{m+1} + O(\Delta x^5) \end{aligned}$$

We then end up with:

$$\frac{U_{j+1}^{m+1} - 2U_j^{m+1} + U_{j-1}^{m+1}}{\Delta x^2} = \partial_x^2 U_j^{m+1} + \frac{1}{12}\Delta x^2 \partial_x^4 U_j^{m+1} + O(\Delta x^3)$$

Next, we consider the time component, which is made of a linear combination of U evaluated at k previous time steps. The coefficients are given by Backward Differentiation Formula:

$$\frac{\frac{1}{\tau}U_j^{m+1}+\frac{\alpha_1}{\tau}U_j^{m}+\cdots+\frac{\alpha_k}{\tau}U_j^{m-k+1}}{\Delta t}$$

For this component, we examine the Taylor expansion of $U_j^{m+1}, U_j^{m-1}, U_j^{m-2}, \cdots,$ U_j^{m-k+1} about U_j^m:

$$U_j^{m+1} = U_j^m + \Delta t \partial_t U_j^m + \frac{1}{2}\Delta t^2 \partial_t^2 U_j^m + O(\Delta t^3)$$

$$U_j^{m-1} = U_j^m - \Delta t \partial_t U_j^m + \frac{1}{2}\Delta t^2 \partial_t^2 U_j^m + O(\Delta t^3)$$

$$U_j^{m-2} = U_j^m - 2\Delta t \partial_t U_j^m + \frac{1}{2}(2\Delta t)^2 \partial_t^2 U_j^m + O(\Delta t^3)$$

$$U_j^{m-3} = U_j^m - 3\Delta t \partial_t U_j^m + \frac{1}{2}(3\Delta t)^2 \partial_t^2 U_j^m + O(\Delta t^3)$$

In general, we have:

$$U_j^{m-k+1} = U_j^m - (k-1)\Delta t \partial_t U_j^m + \frac{1}{2}\Big((k-1)\Delta t\Big)^2 \partial_t^2 U_j^m + O(\Delta t^3)$$

So:

$$\begin{aligned}
\frac{1}{\tau}U_j^{m+1}+\frac{\alpha_1}{\tau}U_j^{m}+\cdots+\frac{\alpha_k}{\tau}U_j^{m-k+1} =& \frac{1}{\tau}\Big(U_j^m + \Delta t \partial_t U_j^m + \frac{1}{2}\Delta t^2 \partial_t^2 U_j^m + O(\Delta t^3)\Big)\\
&+\frac{\alpha_1}{\tau}U_j^m\\
&+\frac{\alpha_2}{\tau}\Big(U_j^m - \Delta t \partial_t U_j^m + \frac{1}{2}\Delta t^2 \partial_t^2 U_j^m + O(\Delta t^3)\Big)\\
&+\frac{\alpha_3}{\tau}\Big(U_j^m - 2\Delta t \partial_t U_j^m + \frac{1}{2}(2\Delta t)^2 \partial_t^2 U_j^m + O(\Delta t^3)\Big)\\
&+\cdots+\\
&+\frac{\alpha_k}{\tau}\Big(U_j^m - (k-1)\Delta t \partial_t U_j^m + \frac{1}{2}\Big((k-1)\Delta t\Big)^2 \partial_t^2 U_j^m + O(\Delta t^3)\Big)
\end{aligned}$$

However, for Backward Differentiation Formula up to order 6:

$$\frac{1}{\tau}+\frac{\alpha_1}{\tau}+\frac{\alpha_2}{\tau}+\cdots+\frac{\alpha_k}{\tau}=0$$

Therefore:

$$\frac{\alpha_1}{\tau}U_j^m+\frac{\alpha_2}{\tau}U_j^m+\cdots+\frac{\alpha_k}{\tau}U_j^m=0$$

So the time component is:

$$\frac{\frac{1}{\tau}U_j^{m+1}+\frac{\alpha_1}{\tau}U_j^m+\cdots+\frac{\alpha_k}{\tau}U_j^{m-k+1}}{\Delta t}=\frac{1}{\tau}\Big(\partial_t U_j^m+\frac{1}{2}\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$
$$+\frac{\alpha_2}{\tau}\Big(-\partial_t U_j^m+\frac{1}{2}\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$
$$+\frac{\alpha_3}{\tau}\Big(-2\partial_t U_j^m+\frac{1}{2}\cdot 4\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$
$$+\cdots+$$
$$+\frac{\alpha_k}{\tau}\Big(-(k-1)\partial_t U_j^m+\frac{1}{2}\cdot(k-1)^2\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$

Now, the truncation errors are:

$$P_{u(x_j,t_m)}-P_{\Delta x,\Delta t,u(x_j,t_m)}=\Big(\partial_t U_j^m-\alpha\partial_x^2 U_j^m\Big)-\Big\{$$
$$\Big[\frac{1}{\tau}\Big(\partial_t U_j^m+\frac{1}{2}\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$
$$+\frac{\alpha_2}{\tau}\Big(-\partial_t U_j^m+\frac{1}{2}\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$
$$+\frac{\alpha_3}{\tau}\Big(-2\partial_t U_j^m+\frac{1}{2}\cdot 4\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)$$
$$+\cdots+$$
$$+\frac{\alpha_k}{\tau}\Big(-(k-1)\partial_t U_j^m+\frac{1}{2}(k-1)^2\Delta t\partial_t^2 U_j^m+O(\Delta t^2)\Big)\Big]$$
$$-\alpha\Big(\partial_x^2 U_j^{m+1}+\frac{1}{12}\Delta x^2\partial_x^4 U_j^{m+1}+O(\Delta x^3)\Big)\Big\}$$

As Δt and Δx approach 0, we are left with:

$$\lim_{\Delta x,\Delta t\to 0}P_{u(x_j,t_m)}-P_{\Delta x,\Delta x,u(x_j,t_m)}=\Big(\partial_t U_j^m-\alpha\partial_x^2 U_j^m\Big)-$$
$$\Big[\Big(\frac{1}{\tau}-\frac{\alpha_2}{\tau}-2\frac{\alpha_3}{\tau}-\cdots-(k-1)\frac{\alpha_k}{\tau}\Big)\partial_t U_j^m-\alpha\Big(\partial_x^2 U_j^{m+1}\Big)\Big]$$

For Backward Differentiation Formula up to order 6,

$$\frac{1}{\tau}-\frac{\alpha_2}{\tau}-2\frac{\alpha_3}{\tau}-\cdots-(k-1)\frac{\alpha_k}{\tau}=1$$

So

$$\Big(\frac{1}{\tau}-\frac{\alpha_2}{\tau}-2\frac{\alpha_3}{\tau}-\cdots-(k-1)\frac{\alpha_k}{\tau}\Big)\partial_t U_j^m=\partial_t U_j^m$$

Not only that, as Δt go to 0, $\partial_x^2 U_j^{m+1}$ gets closer to $\partial_x^2 U_j^m$. Therefore:

$$\lim_{\Delta x, \Delta t \to 0} P_{u(x_j,t_m)} - P_{\Delta x, \Delta x, u(x_j,t_m)} = 0$$

The finite difference schemes given by Backward Differentiation Formula are consistent.

4 Conclusion

In this paper, we propose two types of alternative finite difference schemes, one is given by the explicit Adams-Bashforth and the other one is given by the implicit Backward Differentiation Formula. We successfully justify their consistency by taking the Taylor expansions. In the future, we could possibly extend this research on other types of Partial Differential Equations such as the wave equation and other second-order PDEs or non linear PDEs. Overall, we believe our work brings up a new perspective to the research of finite difference schemes.

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