

Improvement of Stability and Accuracy of Time-Evolution Equation by Implicit Integration

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ABSTRACT—The stability and accuracy of the numerical integration of the time-evolution equation obtained by discretizing an unsteady partial differential equation with respect to space variables has a crucial importance in solving the unsteady partial differential equation numerically. The second and fourth order Runge-Kutta methods are widely used in the numerical integration. However, in some cases, the stability is not sufficient. New implicit methods are proposed to increase stability and accuracy of the solution of the time-evolution equation. Three new implicit methods, that is, implicit method using linear approximation (IMP1), one using parabolic approximation (IMP2) and one using cubic approximation (IMP3) are proposed. In the case of linear problem, IMP1 is identical to the implicit method by Crank and Nicholson. The stability of various methods including Runge-Kutta method is discussed theoretically and numerically, and the numerical examples are shown to show the effectiveness of the Implicit methods. It is proposed that the most practical way to increase both the accuracy and the stability in the solution of unsteady boundary value problems may be to use IMP1 and the smaller spatial mesh size.

Keywords—Time-evolution equation, Implicit Method, Stability, Accuracy

1. INTRODUCTION

If an unsteady partial differential equation is discretized with respect to the space variables, a time-evolution equation with the multi unknown variables is obtained. The stability and accuracy of the numerical integration of the time-evolution equation has a crucial importance in solving the unsteady partial differential equation. Crank and Nicholson [1] and Rosenbrock [2] have discussed not only the stability but also the accuracy theoretically. In the present paper, the same problems are discussed again from the different viewpoint and verified by the numerical results.

The second and fourth order Runge-Kutta methods are widely used in the numerical integration. However, in some cases, the stability is not sufficient. Implicit method is effective in increasing the stability. New implicit methods are proposed to increase stability and accuracy of the solution of the time-evolution equation. The stability of various methods including Runge-Kutta method is discussed theoretically and numerically, and the numerical examples are shown to show the effectiveness of the New Implicit methods.

2. SOLUTION AND PROPERTY OF IMPLICIT METHOD

2.1. Implicit method

Let's consider the numerical integration of a differential equation using a one-dimensional example:

$$\frac{du}{dt} = f(t, u) \text{ in } t > 0 \quad (1)$$

with the initial condition:

$$u = u_0 \text{ at } t = 0. \quad (2)$$

Equation (1) is approximated as

$$\frac{u_{n+1} - u_n}{dt} \approx f(t_n + 0.5dt, u(t_n + 0.5dt)) \text{ at } t = t_n + 0.5dt, \quad (3)$$

where $u_n = u(t_n)$.

If we use an approximation:

$$u(t_n + 0.5dt) \approx 0.5(u_n + u_{n+1}), \quad (4)$$

then, we have

$$u_{n+1} \approx u_n + f(t_n + 0.5dt, 0.5(u_n + u_{n+1}))dt. \quad (5)$$

If $f(t, u)$ is a linear function of u , we can obtain a difference equation to determine u_{n+1} . Even if $f(t, u)$ is a nonlinear function of u , we can solve this equation by iteration. A solution based on the approximation given by Eq. (5) is called an implicit solution.

If approximation:

$$f(t_n + 0.5dt, 0.5(u_n + u_{n+1})) = f(t_n + 0.5dt, u_n + 0.5dt(u_{n+1} - u_n)/dt) \approx f(t_n + 0.5dt, u_n + 0.5dt f(t_n, u_n)) \quad (6)$$

is used, it becomes the second order Runge-Kutta method

$$u_{n+1} \approx u_n + f(t_n + 0.5dt, u_n + 0.5dt f(t_n, u_n))dt \quad (7)$$

The second order Runge-Kutta method is very close to this method but different. Runge-Kutta method is an explicit solution. On the other hand, Euler solution is given by

$$u_{n+1} = u_n + f(t_n, u_n)dt \quad (8)$$

Using Taylor expansion, we have

$$u_{n+1} = u_{n+1/2} + u'_{n+1/2} \frac{dt}{2} + u''_{n+1/2} \frac{dt^2}{8} + O(dt^3), \quad u_n = u_{n+1/2} - u'_{n+1/2} \frac{dt}{2} + u''_{n+1/2} \frac{dt^2}{8} + O(dt^3). \quad (9a, b)$$

Hence, we obtain

$$u_{n+1/2} = \frac{u_n + u_{n+1}}{2} + O(dt^2), \quad u'_{n+1/2} = \frac{u_{n+1} - u_n}{dt} + O(dt^2). \quad (10a, b)$$

From Eq (10), the accuracy of Eq. (4) is estimated as

$$u_{n+1} = u_n + f(t_n + 0.5dt, 0.5(u_n + u_{n+1}))dt + O(dt^3). \quad (11)$$

The second order Runge-Kutta method is also $O(dt^3)$ approximation.

Let's consider the property of the implicit and explicit solutions through examples.

2.1.1. Example 1

A problem is defined as

$$\frac{du}{dt} = f(t, u) = u \text{ in } t > 0, \quad u = 1 \text{ at } t = 0. \quad (12a, b)$$

The exact solution is given by

$$u = e^t. \quad (13)$$

Hence, we have

$$u_{n+1} = e^{(n+1)dt} = e^{dt} u_n. \quad (14)$$

From Eq. (5), the implicit solution is given by

$$u_{n+1} \approx u_n + 0.5(u_n + u_{n+1})dt \text{ or } u_{n+1} \approx \frac{1 + 0.5dt}{1 - 0.5dt} u_n. \quad (15, 16)$$

When $dt \ll 1$

$$u_{n+1} \approx (1 + 0.5dt)(1 + 0.5dt + 0.25dt^2 + \dots)u_n \approx (1 + dt + 0.5dt^2)u_n. \quad (17)$$

From Eq. (7), the solution of the second order Runge-Kutta method is given by

$$u_{n+1} \approx u_n + (u_n + 0.5u_n dt)dt \text{ or } u_{n+1} \approx (1 + dt + 0.5dt^2)u_n. \quad (18, 19)$$

On the other hand, Euler solution is given by

$$u_{n+1} \approx (1 + dt)u_n. \quad (20)$$

In this example, the exact, implicit and Runge-Kutta solutions show the similar tendencies.

2.1.2. Example 2

A problem is defined as

$$\frac{du}{dt} = f(t, u) = -u \text{ in } t > 0, \quad u = 1 \text{ at } t = 0. \quad (21a, b)$$

The exact solution is given by

$$u = e^{-t}. \quad (22)$$

Hence, we have

$$u_{n+1} = e^{-(n+1)dt} = e^{-dt} u_n. \quad (23)$$

From Eq. (5), the implicit solution is given by

$$u_{n+1} \approx u_n - 0.5(u_n + u_{n+1})dt \text{ or } u_{n+1} \approx \frac{1 - 0.5dt}{1 + 0.5dt} u_n. \quad (24, 25)$$

When $dt \ll 1$

$$u_{n+1} \approx (1 - 0.5dt)(1 - 0.5dt + 0.25dt^2 + \dots)u_n \approx (1 - dt + 0.5dt^2)u_n. \quad (26)$$

From Eq. (7), the second order Runge-Kutta solution is given by

$$u_{n+1} \approx u_n - (u_n - 0.5u_n dt)dt \text{ or } u_{n+1} \approx (1 - dt + 0.5dt^2)u_n. \quad (27, 28)$$

On the other hand, Euler solution is given by

$$u_{n+1} \approx (1 - dt)u_n. \quad (29)$$

In this example, the exact, implicit, Euler and Runge-Kutta solutions show the quite different tendencies. When dt tends to ∞ , u_{n+1}/u_n tends to 0 , -1 , $-\infty$ and $-\infty$ for the exact, implicit, Euler and Runge-Kutta solutions, respectively. The implicit solution does not diverge for an arbitrary dt . However, the Euler and Runge-Kutta solutions diverge when $1 - dt < -1$ and $1 - dt - 0.5dt^2 < -1$, respectively. Hence, by making u_{n+1} in f unknown, the stability of the numerical calculation increases drastically, and much larger dt can be used in comparison with explicit methods such as Euler method and Runge-Kutta method.

The stability analysis using Crank-Nicholson's method [1] was conducted for this example in Appendix A. An interesting result is obtained.

2.2. Numerical example

A problem is defined as

$$\frac{du}{dt} = u \text{ in } t > 0, \quad u = 0 \text{ at } t = 0. \quad (30a, b)$$

The exact solution is given by

$$u = e^t - 1. \quad (31)$$

The numerical results are shown in Fig. 1. EUL, IMP and RK2 refer to Euler method, Implicit method and Runge-Kutta method of 2nd order, respectively. Exact means the exact solution. IMP corresponds to IMP1 in section 4.

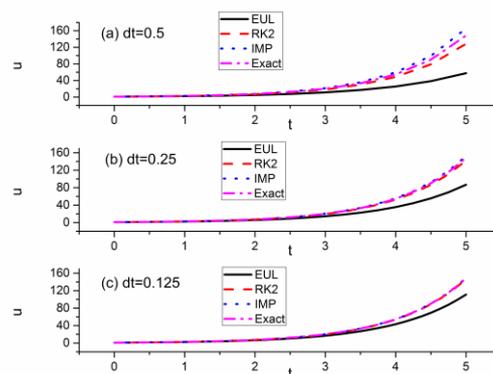


Figure 1: Comparison of various solutions ($du/dt = y$ for $t > 0$, $u(0) = 0$)

The accuracy of the solutions increase as dt becomes smaller. The accuracy of the implicit solution is the highest, and the Runge-Kutta solution is the next. That of the Euler method is much worse.

3. GENERAL LINEAR PROBLEM

3.1. Implicit solution of General linear problem for single unknown variable

If $f(t, u)$ is a linear function of u or $f(t, u) = a(t)u + b(t)$, namely

$$\frac{du}{dt} = a(t)u + b(t), \quad (32)$$

then, we have

$$\frac{u_{n+1} - u_n}{dt} \approx a(t_n + 0.5dt) \frac{u_n + u_{n+1}}{2} + b(t_n + 0.5dt). \quad (33)$$

Rewriting Eq. (33), we derive

$$u_{n+1} = \frac{1}{1 - \frac{1}{2}a(t_n + 0.5dt)dt} \left[\left(1 + \frac{1}{2}a(t_n + 0.5dt)dt \right) u_n + b(t_n + 0.5dt)dt \right]. \quad (34)$$

3.2. Implicit solution of general linear problem for multiple unknown variables

In the case of multiple unknown variables $u_i(t)$, $i = 0, 1, 2, \dots$, the superscript is used to show the time step $t^{(n)}$, $i = 0, 1, 2, \dots$. Hence, $u_i^{(n)}$ refers to $u_i(t^{(n)})$, and $\{u^{(n)}\}$ means a column vector $[u_0^{(n)} \ u_1^{(n)} \ \dots]^T$. A matrix with element A_{ij} , $i = 0, 1, 2, \dots$, $j = 0, 1, 2, \dots$ is denoted by $[A]$.

If the differential equation is given by:

$$[A(t)] \left\{ \frac{du}{dt} \right\} = [a(t)] \{u\} + \{b(t)\}, \quad (35)$$

then, we obtain

$$[A(t^{(n)} + 0.5dt)] \left\{ \frac{u^{(n+1)} - u^{(n)}}{dt} \right\} \approx [a(t^{(n)} + 0.5dt)] \left\{ \frac{u^{(n+1)} + u^{(n)}}{2} \right\} + \{b(t^{(n)} + 0.5dt)\}. \quad (36)$$

Rewriting Eq. (36), we have

$$\left\{ \frac{u^{(n+1)} - u^{(n)}}{dt} \right\} \approx [A(t^{(n)} + 0.5dt)]^{-1} [a(t^{(n)} + 0.5dt)] \left\{ \frac{u^{(n+1)} + u^{(n)}}{2} \right\} + [A(t^{(n)} + 0.5dt)]^{-1} \{b(t^{(n)} + 0.5dt)\}. \quad (37)$$

Hence, we derive

$$\begin{aligned} \{u^{(n+1)}\} &\approx \left[I - \frac{dt}{2} [A(t^{(n)} + 0.5dt)]^{-1} [a(t^{(n)} + 0.5dt)] \right]^{-1} \\ &\cdot \left(\left[I + \frac{dt}{2} [A(t^{(n)} + 0.5dt)]^{-1} [a(t^{(n)} + 0.5dt)] \right] \{u^{(n)}\} + dt [A(t^{(n)} + 0.5dt)]^{-1} \{b(t^{(n)} + 0.5dt)\} \right). \end{aligned} \quad (38)$$

3.2.1. A numerical example:

A problem is defined as

$$\begin{cases} \frac{du_0}{dt} \\ \frac{du_1}{dt} \end{cases} = \begin{bmatrix} 1 & -6 \\ 1 & -4 \end{bmatrix} \begin{cases} u_0 \\ u_1 \end{cases} \text{ in } t > 0, \quad \begin{cases} u_0 \\ u_1 \end{cases} = \begin{cases} 5 \\ 2 \end{cases} \text{ at } t = 0. \quad (39a, b)$$

The exact solution is given by

$$\begin{cases} u_0 \\ u_1 \end{cases} = \begin{cases} 3 \\ 1 \end{cases} e^{-t} + \begin{cases} 2 \\ 1 \end{cases} e^{-2t}. \quad (40)$$

For the exact solution (Exact), we have from Eq. (40), we have

$$\begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases} = \begin{cases} 3 \\ 1 \end{cases} e^{-t^{(n)}} + \begin{cases} 2 \\ 1 \end{cases} e^{-2t^{(n)}} = \begin{bmatrix} 3 & 2 \\ 1 & 1 \end{bmatrix} \begin{cases} e^{-t^{(n)}} \\ e^{-2t^{(n)}} \end{cases}, \quad (41a)$$

$$\begin{cases} u_0^{(n+1)} \\ u_1^{(n+1)} \end{cases} = \begin{cases} 3 \\ 1 \end{cases} e^{-t^{(n)} - dt} + \begin{cases} 2 \\ 1 \end{cases} e^{-2t^{(n)} - 2dt} = \begin{bmatrix} 3e^{-dt} & 2e^{-2dt} \\ e^{-dt} & e^{-2dt} \end{bmatrix} \begin{cases} e^{-t^{(n)}} \\ e^{-2t^{(n)}} \end{cases}. \quad (41b)$$

Hence, we obtain

$$\begin{aligned} \begin{cases} u_0^{(n+1)} \\ u_1^{(n+1)} \end{cases} &= \begin{bmatrix} 3e^{-dt} & 2e^{-2dt} \\ e^{-dt} & e^{-2dt} \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 1 & 1 \end{bmatrix}^{-1} \begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases} = \begin{bmatrix} 3e^{-dt} & 2e^{-2dt} \\ e^{-dt} & e^{-2dt} \end{bmatrix} \begin{bmatrix} 1 & -2 \\ -1 & 3 \end{bmatrix} \begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases} \\ &= \begin{bmatrix} 3e^{-dt} - 2e^{-2dt} & -6e^{-dt} + 6e^{-2dt} \\ e^{-dt} - e^{-2dt} & -2e^{-dt} + 3e^{-2dt} \end{bmatrix} \begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases} \end{aligned} \quad (42a)$$

$$\approx \begin{bmatrix} 1 + dt - 2.5dt^2 & -6dt + 9dt^2 \\ dt - 1.5dt^2 & 1 - 4dt + 5dt^2 \end{bmatrix} \begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases}. \quad (42b)$$

For the implicit solution (IMP1), $[A]$, $[a]$ and $\{b\}$ in Eq. (38), are given as

$$[A] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, [a] = \begin{bmatrix} 1 & -6 \\ 1 & -4 \end{bmatrix}, \{b\} = 0. \quad (43)$$

Hence, we have

$$\begin{aligned} \begin{cases} u_0^{(n+1)} \\ u_1^{(n+1)} \end{cases} &\approx \left[I - \frac{dt}{2} \begin{bmatrix} 1 & -6 \\ 1 & -4 \end{bmatrix} \right]^{-1} \left[I + \frac{dt}{2} \begin{bmatrix} 1 & -6 \\ 1 & -4 \end{bmatrix} \right] \begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases} \\ &= \frac{1}{1 + 1.5dt + 0.5dt^2} \begin{bmatrix} 1 + 2.5dt - 0.5dt^2 & -6dt \\ dt & 1 - 2.5dt - 0.5dt^2 \end{bmatrix} \begin{cases} u_0^{(n)} \\ u_1^{(n)} \end{cases} \end{aligned} \quad (44a)$$

$$\approx \begin{bmatrix} 1 + dt - 3.625dt^2 & -6dt + 9dt^2 \\ dt - 1.5dt^2 & 1 - 4dt + 3.875dt^2 \end{bmatrix} \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix}. \quad (44b)$$

For Euler solution (EUL), we have

$$\begin{Bmatrix} u_0^{(n+1)} \\ u_1^{(n+1)} \end{Bmatrix} \approx \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix} + dt [a_{ij}] \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix} = \begin{bmatrix} 1 + dt & -6dt \\ dt & 1 - 4dt \end{bmatrix} \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix}. \quad (45)$$

For the second order Runge-Kutta solution (RK2), we have

$$\begin{Bmatrix} u_0^{(n+1)} \\ u_1^{(n+1)} \end{Bmatrix} \approx \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix} + dt [a_{ij}] \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix} + 0.5dt [a_{ij}] \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix} = \begin{bmatrix} 1 + dt - 2.5dt^2 & -6dt + 9dt^2 \\ dt - 1.5dt^2 & 1 - 4dt + 5dt^2 \end{bmatrix} \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix}. \quad (46)$$

From Eqs. (42b), (44b), (45) and (46), $[u_0^{(n+1)} \ u_1^{(n+1)}]^T$ is expressed by $[u_0^{(n)} \ u_1^{(n)}]^T$ as

$$\begin{Bmatrix} u_0^{(n+1)} \\ u_1^{(n+1)} \end{Bmatrix} \approx \begin{bmatrix} C_{00} & C_{01} \\ C_{10} & C_{01} \end{bmatrix} \begin{Bmatrix} u_0^{(n)} \\ u_1^{(n)} \end{Bmatrix}. \quad (47)$$

In Fig. 2, C_{ij} s are compared in various solutions. In Fig. 3-5, u_0 and u_1 are compared in various solutions. The accuracy of the solution is higher in the order of IMP1, RK2 and EUL.

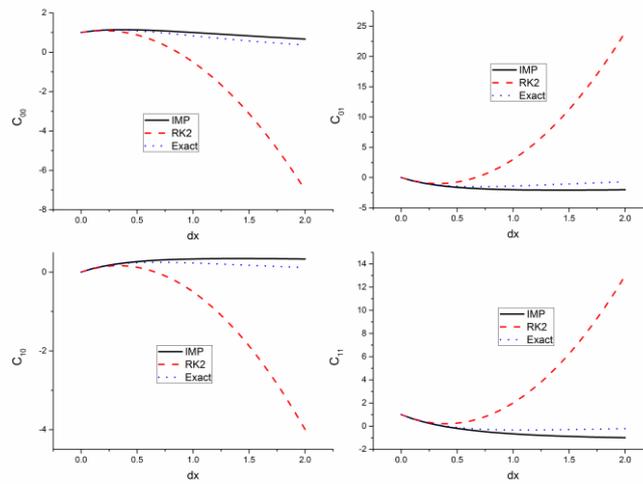


Figure 2: Stability criteria of numerical procedure

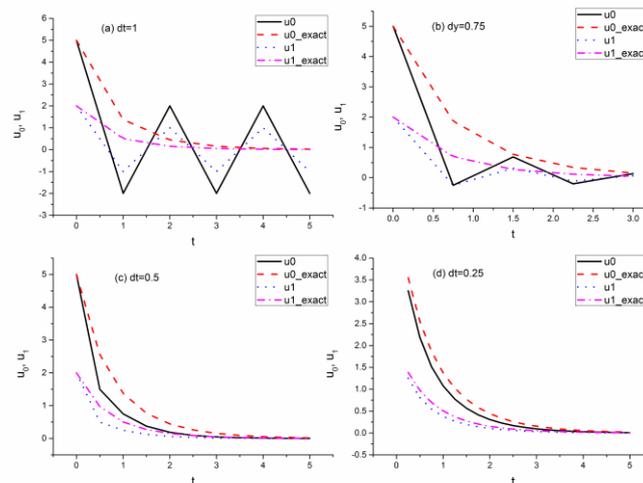


Figure 3: EUL

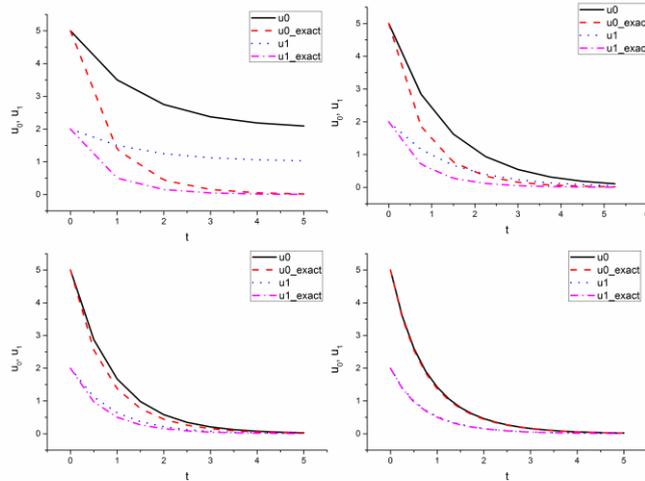


Figure 4: RK2

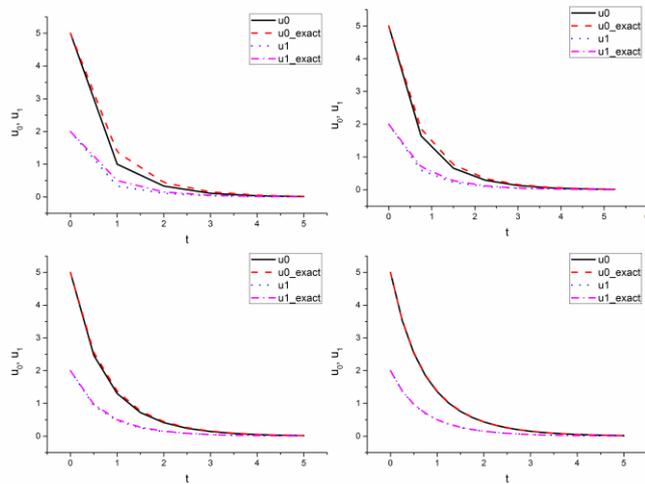


Figure 5: IMP1

4. A NEW IMPLICIT METHOD

From Eq. (1), we have

$$u_{n+1} = u_n + \int_{t_n}^{t_{n+1}} \frac{du}{dt} dt = u_n + \int_{t_n}^{t_{n+1}} f(t, u(t)) dt. \quad (48)$$

4.1. Constant approximation

If $f(t, u(t))$ is approximated by a constant in $t_n \leq t \leq t_{n+1}$:

$$f(t, u(t)) \approx f(t_{n+1/2}, u_{n+1/2}), \quad (49)$$

where $t_{n+1/2}$ and $u_{n+1/2}$ are defined as $t_{n+1/2} = t_n + 0.5dt$ and $u_{n+1/2} = u(t_{n+1/2})$, respectively, then, we have

$$\int_{t_n}^{t_{n+1}} f(t, u(t)) dx \approx dt f(t_{n+1/2}, u_{n+1/2}) \approx dt f(t_{n+1/2}, 0.5(u_n + u_{n+1})). \quad (50)$$

Substituting this into Eq. (50), we obtain

$$u_{n+1} \approx u_n + dt f(t_{n+1/2}, 0.5(u_n + u_{n+1})). \quad (51)$$

This approximation is equal to Eq. (5).

4.2. Linear approximation

If $f(t, u(t))$ is approximated by linear function of t in $t_n \leq t \leq t_{n+1}$:

$$f(t, u(t)) \approx f(t_n, u_n) \frac{(t - t_{n+1})}{(t_n - t_{n+1})} + f(t_{n+1}, u_{n+1}) \frac{(t - t_n)}{(t_{n+1} - t_n)}, \quad (52)$$

then, we have

$$\int_{t_n}^{t_{n+1}} f(t, u(t)) dt \approx \frac{dt}{2} [f(t_n, u_n) + f(t_{n+1}, u_{n+1})]. \quad (53)$$

Substituting this into Eq. (48), we obtain

$$u_{n+1} \approx u_n + \frac{dt}{2} [f(t_n, u_n) + f(t_{n+1}, u_{n+1})]. \quad (54)$$

u_{n+1} can be obtained by iteration.

4.3. Parabolic approximation

If $f(t, u(t))$ is approximated by the second order function of t in $t_n \leq t \leq t_{n+1}$:

$$f(t, u(x)) \approx f(t_n, u_n) \frac{(t - t_{n+1/2})(t - t_{n+1})}{(t_n - t_{n+1/2})(t_n - t_{n+1})} + f(t_{n+1/2}, u_{n+1/2}) \frac{(t - t_n)(t - t_{n+1})}{(t_{n+1/2} - t_n)(t_{n+1/2} - t_{n+1})} + f(t_{n+1}, u_{n+1}) \frac{(t - t_n)(t - t_{n+1/2})}{(t_{n+1} - t_n)(t_{n+1} - t_{n+1/2})}, \quad (55)$$

then, we have

$$\int_{t_n}^{t_{n+1}} f(t, u(t)) dt \approx \frac{dt}{6} [f(t_n, u_n) + 4f(t_{n+1/2}, u_{n+1/2}) + f(t_{n+1}, u_{n+1})]. \quad (56)$$

If $u(x)$ is approximated by

$$u(t) \approx u_n + f(t_n, u_n)(t - t_n) + \frac{1}{dt^2} [u_{n+1} - u_n - f(t_n, u_n)dt](t - t_n)^2, \quad (57)$$

we have

$$u(t_n) = u_n, \quad \left[\frac{du}{dt} \right]_{t=t_n} = f(t_n, u_n) \quad \text{and} \quad u(t_{n+1}) = u_{n+1}. \quad (58)$$

Hence, we obtain

$$u_{n+1/2} \approx u_n + f(t_n, u_n) \frac{dt}{2} + \frac{1}{4} [u_{n+1} - u_n - f(t_n, u_n)dt] = \frac{3}{4} u_n + f(t_n, u_n) \frac{dt}{4} + \frac{1}{4} u_{n+1}. \quad (59)$$

Substituting Eq. (56) into Eq. (48), we derive

$$u_{n+1} \approx u_n + \frac{dt}{6} [f(t_n, u_n) + 4f(t_{n+1/2}, u_{n+1/2}) + f(t_{n+1}, u_{n+1})], \quad (60)$$

where $u_{n+1/2}$ is approximated by Eq. (59). u_{n+1} may be obtained by iteration.

4.4. Cubic approximation

If $f(t, u(t))$ is approximated by the third order function of t in $t_n \leq t \leq t_{n+1}$:

$$f(t, u(t)) \approx f_n \frac{(t - t_{n+1/3})(t - t_{n+2/3})(t - t_{n+1})}{(t_n - t_{n+1/3})(t_n - t_{n+2/3})(t_n - t_{n+1})} + f_{n+1/3} \frac{(t - t_n)(t - t_{n+2/3})(t - t_{n+1})}{(t_{n+1/3} - t_n)(t_{n+1/3} - t_{n+2/3})(t_{n+1/3} - t_{n+1})} + f_{n+2/3} \frac{(t - t_n)(t - t_{n+1/3})(t - t_{n+1})}{(t_{n+2/3} - t_n)(t_{n+2/3} - t_{n+1/3})(t_{n+2/3} - t_{n+1})} + f_{n+1} \frac{(t - t_n)(t - t_{n+1/3})(t - t_{n+2/3})}{(t_{n+1} - t_n)(t_{n+1} - t_{n+1/3})(t_{n+1} - t_{n+2/3})}, \quad (61)$$

where

$$t_{n+1/3} = t_n + \frac{1}{3} dt, \quad t_{n+2/3} = t_n + \frac{2}{3} dt, \quad (62a)$$

$$u_n = u(t_n), \quad u_{n+1/3} = u(t_{n+1/3}), \quad u_{n+2/3} = u(t_{n+2/3}), \quad u_{n+1} = u(t_{n+1}) \quad (62b)$$

$$f_n = f(t_n, u_n), \quad f_{n+1/3} = f(t_{n+1/3}, u_{n+1/3}), \quad f_{n+2/3} = f(t_{n+2/3}, u_{n+2/3}), \quad f_{n+1} = f(t_{n+1}, u_{n+1}), \quad (62c)$$

then, we have (see Appendix B)

$$\int_{t_n}^{t_{n+1}} f(t, u(t)) dt \approx F_{n,0} f_n + F_{n,1/3} f_{n+1/3} + F_{n,2/3} f_{n+2/3} + F_{n,1} f_{n+1}, \quad (63)$$

where

$$I(a, b, m_1, m_2, m_3) = \left[\frac{1}{4}(b^4 - a^4) - \frac{1}{3}(m_1 + m_2 + m_3)(b^3 - a^3) + \frac{1}{2}(m_1 m_2 + m_2 m_3 + m_3 m_1)(b^2 - a^2) - m_1 m_2 m_3(b - a) \right], \quad (64a)$$

$$F_{n,0} = \frac{I(t_n, t_{n+1}, t_{n+1/3}, t_{n+2/3}, t_{n+1})}{(t_n - t_{n+1/3})(t_n - t_{n+2/3})(t_n - t_{n+1})} = -\frac{9}{2dt^3} I(t_n, t_{n+1}, t_{n+1/3}, t_{n+2/3}, t_{n+1}), \quad (64b)$$

$$F_{n,1/3} = \frac{I(t_n, t_{n+1}, t_n, t_{n+2/3}, t_{n+1})}{(t_{n+1/3} - t_n)(t_{n+1/3} - t_{n+2/3})(t_{n+1/3} - t_{n+1})} = \frac{27}{2dt^3} I(t_n, t_{n+1}, t_n, t_{n+2/3}, t_{n+1}), \quad (64c)$$

$$F_{n,2/3} = \frac{I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+1})}{(t_{n+2/3} - t_n)(t_{n+2/3} - t_{n+1/3})(t_{n+2/3} - t_{n+1})} = -\frac{27}{2dt^3} I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+1}), \quad (64d)$$

$$F_{n,1} = \frac{I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+2/3})}{(t_{n+1} - t_n)(t_{n+1} - t_{n+1/3})(t_{n+1} - t_{n+2/3})} = \frac{9}{2dt^3} I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+2/3}). \quad (64e)$$

If $u(t)$ is approximated by a cubic function:

$$u(t) \approx u(t_n) + f(t_n, u(t_n))(t - t_n) + p_n(t - t_n)^2 + q_n(t - t_n)^3, \quad (65)$$

then, we have

$$u_{n+1/3} \approx u_n + f_n \frac{dt}{3} + p_n \frac{dt^2}{9} + q_n \frac{dt^3}{27}, \quad u_{n+2/3} \approx u_n + f_n \frac{2dt}{3} + p_n \frac{4dt^2}{9} + q_n \frac{8dt^3}{27}, \quad (66a, b)$$

where

$$p_n = \frac{1}{dt^2} (3u_{n+1} - 3u_n - 2f_n dt - f_{n+1} dt), \quad q_n = -\frac{1}{dt^3} (2u_{n+1} - 2u_n - f_n dt - f_{n+1} dt). \quad (67a, b)$$

Eq. (67) is obtained by solving

$$u(t_{n+1}) = u(t_n) + f(t_n, u(t_n))dt + p_n dt^2 + q_n dt^3, \quad f(t_{n+1}, u(t_{n+1})) = f(t_n, u(t_n)) + 2p_n dt + 3q_n dt^2. \quad (68a, b)$$

$u(t_{n+1})$ is approximated by

$$u(t_{n+1}) \approx u(t_n) + F_{n,0} f_n + F_{n,1/3} f_{n+1/3} + F_{n,2/3} f_{n+2/3} + F_{n,1} f_{n+1}. \quad (69)$$

4.5. Numerical example

4.5.1. Linear case

We check the effect of the implicit method by a linear problem such as

$$du/dt = -u \quad \text{in } t > 0, \quad u = 1 \quad \text{at } t = 0. \quad (70a, b)$$

The exact solution is given by

$$u = e^{-t}. \quad (71)$$

Various numerical results are compared in Table 1. In the table, EUL, RK2, RK4, IMP1, IMP2, IMP3 and Exact refer to Euler method, 2nd order Runge-Kutta method, 4th order Runge-Kutta method, Implicit method using linear approximation, Implicit method using parabolic approximation, Implicit method using cubic approximation and exact solution, respectively. The accuracy is higher in the order of column.

Table 1: Comparison of numerical results of linear problem

| t | EUL | RK2 | IMP1 | IMP2 | RK4 | IMP3 | Exact |
|-----|----------|----------|----------|----------|----------|----------|----------|
| 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 0.5 | 0.5 | 0.625 | 0.600006 | 0.607143 | 0.606771 | 0.606554 | 0.606531 |
| 1 | 0.25 | 0.390625 | 0.360013 | 0.368623 | 0.368171 | 0.367911 | 0.367879 |
| 1.5 | 0.125 | 0.244141 | 0.216014 | 0.223807 | 0.223395 | 0.22316 | 0.22313 |
| 2 | 0.0625 | 0.152588 | 0.129594 | 0.135882 | 0.13555 | 0.13536 | 0.135335 |
| 2.5 | 0.03125 | 0.095367 | 0.077748 | 0.082499 | 0.082248 | 0.082103 | 0.082085 |
| 3 | 0.015625 | 0.059605 | 0.046644 | 0.050088 | 0.049905 | 0.0498 | 0.049787 |
| 3.5 | 0.007813 | 0.037253 | 0.027998 | 0.030412 | 0.030281 | 0.030206 | 0.030197 |
| 4 | 0.003906 | 0.023283 | 0.016806 | 0.018465 | 0.018374 | 0.018322 | 0.018316 |
| 4.5 | 0.001953 | 0.014552 | 0.010066 | 0.011212 | 0.011149 | 0.011113 | 0.011109 |
| 5 | 0.000977 | 0.009095 | 0.006029 | 0.006807 | 0.006765 | 0.00674 | 0.006738 |
| 5.5 | 0.000488 | 0.005684 | 0.003611 | 0.004132 | 0.004105 | 0.004088 | 0.004087 |
| 6 | 0.000244 | 0.003553 | 0.002182 | 0.002508 | 0.002491 | 0.002479 | 0.002479 |
| 6.5 | 0.000122 | 0.00222 | 0.001318 | 0.001522 | 0.001511 | 0.001504 | 0.001503 |
| 7 | 0.000061 | 0.001388 | 0.000796 | 0.000926 | 0.000917 | 0.000912 | 0.000912 |
| 7.5 | 0.000031 | 0.000867 | 0.000465 | 0.000563 | 0.000556 | 0.000554 | 0.000553 |

| | | | | | | | |
|-----|----------|----------|----------|----------|----------|----------|----------|
| 8 | 0.000015 | 0.000542 | 0.00027 | 0.000342 | 0.000338 | 0.000336 | 0.000335 |
| 8.5 | 0.000008 | 0.000339 | 0.000156 | 0.000208 | 0.000205 | 0.000204 | 0.000203 |
| 9 | 0.000004 | 0.000212 | 0.000107 | 0.000125 | 0.000124 | 0.000124 | 0.000123 |
| 9.5 | 0.000002 | 0.000132 | 0.000057 | 0.000075 | 0.000075 | 0.000074 | 0.000075 |
| 10 | 0.000001 | 0.000083 | 0.000007 | 0.000045 | 0.000046 | 0.000045 | 0.000045 |

4.5.2. Nonlinear example

We check the effect of the implicit method by nonlinear problem such as

$$du/dt = u^2 \text{ in } t > 0, \quad u = -1 \text{ at } t = 0. \quad (72a, b)$$

The exact solution is given by

$$u = \frac{-1}{t+1}. \quad (73)$$

Various numerical results are compared in Table 1. The accuracy is higher in the order of column.

Table 2: Comparison of numerical results of nonlinear problem

| <i>t</i> | EUL | RK2 | IMP1 | IMP2 | IMP3 | RK4 | Exact |
|----------|----------|----------|----------|----------|----------|----------|----------|
| 0 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| 0.5 | -0.5 | -0.71875 | -0.65683 | -0.66993 | -0.66703 | -0.66668 | -0.66667 |
| 1 | -0.375 | -0.54494 | -0.49188 | -0.50244 | -0.50025 | -0.50003 | -0.5 |
| 1.5 | -0.30469 | -0.43416 | -0.39381 | -0.40174 | -0.40017 | -0.40003 | -0.4 |
| 2 | -0.25827 | -0.35926 | -0.32859 | -0.3346 | -0.33346 | -0.33335 | -0.33333 |
| 2.5 | -0.22492 | -0.3058 | -0.28198 | -0.28668 | -0.28581 | -0.28573 | -0.28571 |
| 3 | -0.19962 | -0.26592 | -0.247 | -0.25075 | -0.25007 | -0.25001 | -0.25 |
| 3.5 | -0.1797 | -0.23511 | -0.21976 | -0.22282 | -0.22228 | -0.22223 | -0.22222 |
| 4 | -0.16355 | -0.21062 | -0.19796 | -0.20049 | -0.20005 | -0.20001 | -0.2 |
| 4.5 | -0.15018 | -0.19072 | -0.1801 | -0.18222 | -0.18186 | -0.18183 | -0.18182 |
| 5 | -0.1389 | -0.17422 | -0.1652 | -0.16701 | -0.1667 | -0.16667 | -0.16667 |
| 5.5 | -0.12926 | -0.16034 | -0.15257 | -0.15414 | -0.15387 | -0.15385 | -0.15385 |
| 6 | -0.1209 | -0.14849 | -0.14175 | -0.14311 | -0.14288 | -0.14286 | -0.14286 |
| 6.5 | -0.11359 | -0.13827 | -0.13236 | -0.13356 | -0.13335 | -0.13334 | -0.13333 |
| 7 | -0.10714 | -0.12936 | -0.12413 | -0.1252 | -0.12502 | -0.125 | -0.125 |
| 7.5 | -0.1014 | -0.12153 | -0.11686 | -0.11782 | -0.11766 | -0.11765 | -0.11765 |
| 8 | -0.09626 | -0.11459 | -0.11041 | -0.11127 | -0.11113 | -0.11111 | -0.11111 |
| 8.5 | -0.09163 | -0.10839 | -0.10462 | -0.1054 | -0.10528 | -0.10527 | -0.10526 |
| 9 | -0.08743 | -0.10283 | -0.09942 | -0.10013 | -0.10001 | -0.1 | -0.1 |
| 9.5 | -0.08361 | -0.09781 | -0.09471 | -0.09535 | -0.09525 | -0.09524 | -0.09524 |
| 10 | -0.08011 | -0.09326 | -0.09042 | -0.09101 | -0.09092 | -0.09091 | -0.09091 |

5. APPLICATION OF NEW IMPLICIT METHODS TO SOLUTION OF PARTIAL DIFFERENTIAL EQUATION

5.1. Diffusion equation

5.1.1. Diffusion in a still fluid

The initial-boundary value problem of Diffusion equation is defined by

$$\frac{\partial u}{\partial t} = v \frac{\partial^2 u}{\partial x^2} \text{ in } 0 < x < L, \quad (74)$$

$$u(x,0) = f(x); \quad u(0,t) = U_0, \quad u(L,t) = U_L. \quad (75a, b)$$

We divide the computational region into *N* elements $x_i < x < x_{i+1}$, where

$$dx = \frac{L}{N}; \quad x_i = idx, \quad i = 0,1,\dots,N. \quad (76a, b)$$

We use the difference operations to approximate the spatial derivatives. If we denote $u(x_i,t)$ as $u_i(t)$, then, we have

$$\frac{du_i}{dt} = v \frac{1}{dx^2} (u_{i+1} - 2u_i + u_{i-1}), \quad i = 0,1,\dots,N, \quad (77)$$

$$u_i(0) = f(x_i); \quad u_0(t) = \text{const} = U_0, \quad u_N(t) = \text{const} = U_L. \quad (78a, b)$$

Equations (77) and (78) can be rewritten as

$$\left\{ \frac{du}{dt} \right\} = \frac{\nu}{dx^2} [a] \{u\}, \quad (79)$$

where

$$\{u\} = [u_1 \quad u_1 \quad \cdots \quad u_{N-1}]^T; \quad a_{i,j} = \begin{cases} 1 & \text{for } j = i - 1 \text{ \& } i + 1 \\ -2 & \text{for } j = i \\ 0 & \text{otherwise} \end{cases} \quad \text{for } i = 1, 2, \dots, N - 1. \quad (80a, b)$$

From Eq. (79), the following time-progressive equations for Euler method (EUL), Implicit method using linear approximation (IMP1), Runge-Kutta method of the 2nd order (RK2) and Implicit method using parabolic approximation (IMP2) are given below, where u_i at time step n is denoted as $u_i^{(n)}$.

EUL:

$$\{u^{(n+1)}\} = [I] \{u^{(n)}\} + \frac{\nu dt}{dx^2} [a] \{u^{(n)}\} + \frac{\nu dt}{dx^2} \{\delta_1\} U_0(t) + \frac{\nu dt}{dx^2} \{\delta_{N-1}\} U_L(t), \quad (81)$$

where $\{\delta_1\} = [1 \quad 0 \quad \cdots \quad 0]$ and $\{\delta_{N-1}\} = [0 \quad \cdots \quad 0 \quad 1]$.

IMP1:

$$\{u^{(n+1)}\} = \{u^{(n)}\} + \frac{\nu dt}{dx^2} [a] \frac{1}{2} \{u^{(n)} + u^{(n+1)}\} + \frac{\nu dt}{dx^2} \{\delta_1\} U_0((n+0.5)t) + \frac{\nu dt}{dx^2} \{\delta_{N-1}\} U_L((n+0.5)t) \quad (82a)$$

or

$$\left[I - \frac{\nu dt}{2dx^2} a \right] \{u^{(n+1)}\} = \left[I + \frac{\nu dt}{2dx^2} \right] \{u^{(n)}\} + \frac{\nu dt}{dx^2} \{\delta_1\} U_0((n+0.5)t) + \frac{\nu dt}{dx^2} \{\delta_{N-1}\} U_L((n+0.5)t). \quad (82b)$$

RK2:

$$\{u^{(n+1)}\} = \{u^{(n)}\} + \frac{\nu dt}{dx^2} [a] \{u^{(n+1/2)}\} + \frac{\nu dt}{dx^2} \{\delta_1\} U_0((n+0.5)t) + \frac{\nu dt}{dx^2} \{\delta_{N-1}\} U_L((n+0.5)t), \quad (83a)$$

$$\{u^{(n+1/2)}\} = \{u^{(n)}\} + \frac{1}{2} \frac{\nu dt}{dx^2} [a] \{u^{(n)}\} + \frac{1}{2} \frac{\nu dt}{dx^2} \{\delta_1\} U_0(nt) + \frac{1}{2} \frac{\nu dt}{dx^2} \{\delta_{N-1}\} U_L(nt). \quad (83b)$$

IMP2:

$$\{u^{(n+1/2)}\} = \frac{3}{4} \{u^{(n)}\} + \frac{\nu dt}{dx^2} [a] \frac{1}{4} \{u^{(n)}\} + \frac{1}{4} \{u^{(n+1)}\}, \quad (84a)$$

$$\begin{aligned} \{u^{(n+1)}\} = \{u^{(n)}\} + \frac{\nu dt}{dx^2} [a] \frac{1}{6} \{u^{(n)} + 4u^{(n+1/2)} + u^{(n+1)}\} + \frac{\nu dt}{dx^2} \{\delta_1\} \frac{1}{6} (U_0(nt) + 4U_0((n+0.5)t) + U_0((n+1)t)) \\ + \frac{\nu dt}{dx^2} \{\delta_{N-1}\} \frac{1}{6} (U_L(nt) + 4U_L((n+0.5)t) + U_L((n+1)t)) \end{aligned} \quad (84b)$$

or eliminating $\{u^{(n+1/2)}\}$

$$\begin{aligned} \left[I - \frac{\nu dt}{3dx^2} a \right] \{u^{(n+1)}\} = \left[I + \frac{2\nu dt}{3dx^2} a + \frac{1}{6} \left(\frac{\nu dt}{dx^2} \right)^2 a^2 \right] \{u^{(n)}\} + \frac{\nu dt}{dx^2} \{\delta_1\} \frac{1}{6} (U_0(nt) + 4U_0((n+0.5)t) + U_0((n+1)t)) \\ + \frac{\nu dt}{dx^2} \{\delta_{N-1}\} \frac{1}{6} (U_L(nt) + 4U_L((n+0.5)t) + U_L((n+1)t)). \end{aligned} \quad (85)$$

The initial condition is given by

$$u_i^{(0)} = f(x_i) \quad \text{for } i = 0, 1, \dots, N. \quad (86)$$

The exact solution of the initial-boundary value problem, Eqs. (74) and (75) is given by

$$u(x, t) = U_0 + (U_L - U_0) \frac{x}{L} + \sum_{m=1}^{\infty} a_m \exp \left[-\nu \left(\frac{m\pi}{L} \right)^2 t \right] \sin \left(\frac{m\pi}{L} x \right), \quad (87a)$$

where

$$\alpha_m = \frac{2}{L} \int_0^L f(x) \sin \left(\frac{m\pi}{L} x \right) dx - \frac{2}{m\pi} [U_0(1 - (-1)^m) - (U_L - U_0)(-1)^m]. \quad (87b)$$

The numerical results are shown in Tables 3 and Fig. 6. In Tables 3, ν is the kinematic viscosity, and symbols \bigcirc and \times means whether the calculation is conducted normally or diverged, respectively. The stability of IMP1 is much higher than EUL and RK2. In Fig. 6, the accuracy is compared among EUL, RK2 and IMP1. The accuracy of IMP1 is high.

Table 3: $f = 0, U_0 = 1, U_L = 0, L=1, \nu = 0.089, t_{\max} = 2.5$

| | EUL | | | RK2 | | | IMP1 | | |
|-------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| | $N=20$ | $N=40$ | $N=80$ | $N=20$ | $N=40$ | $N=80$ | $N=20$ | $N=40$ | $N=80$ |
| $dt=0.0025$ | ○ | ○ | × | ○ | ○ | × | ○ | ○ | ○ |
| $dt=0.005$ | ○ | × | × | ○ | × | × | ○ | ○ | ○ |
| $dt=0.01$ | ○ | × | × | ○ | × | × | ○ | ○ | ○ |
| $dt=0.1$ | × | × | × | × | × | × | ○ | ○ | ○ |
| $dt=1$ | × | × | × | × | × | × | ○ | ○ | ○ |

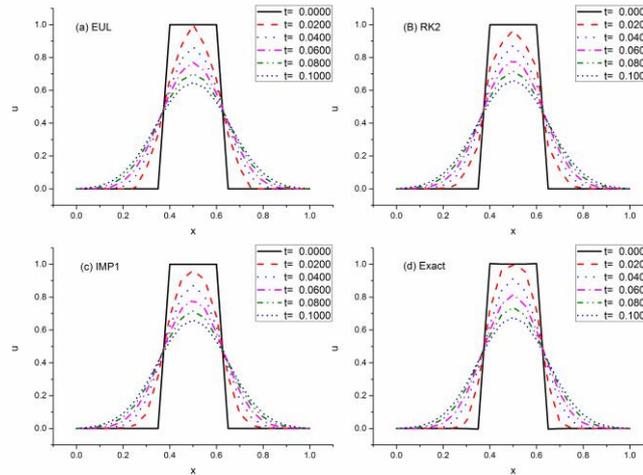


Figure 6: Comparison of accuracy of the solutions by IMP1 ($f = \text{hat}, U_0 = 0, U_L = 0, L = 1, N = 20, dt = 0.01, t = 1, \nu = 0.089$)

5.1.2. Diffusion in a flow with uniform flow

If there is a flow in the fluid, the initial-boundary value problem of Diffusion equation is defined by

$$\frac{\partial u}{\partial t} + V \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \text{ in } 0 < x < L, \quad (88)$$

$$u(x,0) = f(x); \quad u(0,t) = 0, \quad u(L,t) = 0, \quad (89a, b)$$

where V is the velocity of the uniform flow.

We divide the computational region into N elements as given by Eq. (76). We use the difference operations to approximate the spatial derivatives. If we denote $u(x_i, t)$ as $u_i(t)$, then, we have

$$\frac{du_i}{dt} = -V \frac{1}{2dx} (u_{i+1} - u_{i-1}) + \nu \frac{1}{dx^2} (u_{i+1} - 2u_i + u_{i-1}), \quad i = 0, 1, \dots, N, \quad (90)$$

$$u_i(0) = f(x_i); \quad u_0(t) = 0, \quad u_N(t) = 0. \quad (91a, b)$$

Equations (90) and (91) can be rewritten as

$$\left\{ \frac{du}{dt} \right\} = -\frac{V}{2dx} [b]\{u\} + \frac{\nu}{dx^2} [a]\{u\}, \quad (92)$$

where $\{u\}$ and $[a]$ are given by Eq. (80), and $[b]$ is defined by

$$b_{ij} = \begin{cases} -1 & \text{for } j = i - 1 \\ +1 & \text{for } j = i + 1 \text{ for } i = 1, 2, \dots, N - 1. \\ 0 & \text{otherwise} \end{cases} \quad (93)$$

From Eq. (92), the following time-progressive equations for Euler method (EUL), Implicit method using linear approximation (IMP1), Runge-Kutta method of the 2nd order (RK2) and Implicit method using parabolic approximation (IMP2) are given below, where u_i at time step n is denoted as $u_i^{(n)}$.

EUL:

$$\{u^{(n+1)}\} = [I]\{u^{(n)}\} + \left(-\frac{Vdt}{2dx}[b] + \frac{vdt}{dx^2}[a]\right)\{u^{(n)}\}, \quad (94)$$

where $\{\delta_1\} = [1 \ 0 \ \dots \ 0]$ and $\{\delta_{N-1}\} = [0 \ \dots \ 0 \ 1]$.

IMP1:

$$\{u^{(n+1)}\} = [I]\{u^{(n)}\} + \left(-\frac{Vdt}{2dx}[b] + \frac{vdt}{dx^2}[a]\right)\frac{1}{2}\{u^{(n)} + u^{(n+1)}\}, \quad (95a)$$

or

$$\left[I + \frac{Vdt}{4dx}b - \frac{vdt}{2dx^2}a\right]\{u^{(n+1)}\} = \left[I - \frac{Vdt}{4dx}b + \frac{vdt}{2dx^2}a\right]\{u^{(n)}\}. \quad (95b)$$

RK2:

$$\{u^{(n+1)}\} = \{u^{(n)}\} + \left(-\frac{Vdt}{2dx}[b] + \frac{vdt}{dx^2}[a]\right)\{u^{(n+1/2)}\}, \quad (96a)$$

$$\{u^{(n+1/2)}\} = \{u^{(n)}\} + \frac{1}{2}\left(-\frac{Vdt}{2dx}[b] + \frac{vdt}{dx^2}[a]\right)\{u^{(n)}\}. \quad (96b)$$

IMP2:

$$\{u^{(n+1/2)}\} = \frac{3}{4}\{u^{(n)}\} + \left(-\frac{Vdt}{2dx}[b] + \frac{vdt}{dx^2}[a]\right)\frac{1}{4}\{u^{(n)}\} + \frac{1}{4}\{u^{(n+1)}\}, \quad (97a)$$

$$\{u^{(n+1)}\} = \{u^{(n)}\} + \left(-\frac{Vdt}{2dx}[b] + \frac{vdt}{dx^2}[a]\right)\frac{1}{6}\{u^{(n)} + 4u^{(n+1/2)} + u^{(n+1)}\} \quad (97b)$$

or eliminating $\{u^{(n+1/2)}\}$

$$\left[I - \frac{1}{3}\left(-\frac{Vdt}{2dx}b + \frac{vdt}{dx^2}a\right)\right]\{u^{(n+1)}\} = \left[I + \frac{2}{3}\left(-\frac{Vdt}{2dx}b + \frac{vdt}{dx^2}a\right) + \frac{1}{6}\left(-\frac{Vdt}{2dx}b + \frac{vdt}{dx^2}a\right)^2\right]\{u^{(n)}\}. \quad (98)$$

The initial condition is given by

$$u_i^{(0)} = f(x_i) \text{ for } i = 0, 1, \dots, N. \quad (99)$$

The exact solution of the initial-boundary value problem, Eqs. (88) and (89), is given by

$$u(x, t) = \sum_{m=1}^{\infty} a_m \exp\left[-v\left(\frac{m\pi}{L}\right)^2 t\right] \sin\left(\frac{m\pi}{L}(x - Vt)\right), \quad (100a)$$

where

$$a_m = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{m\pi}{L}x\right) dx. \quad (100b)$$

The numerical results are shown in Figs. 7, 8 and 9. The initial condition $f(x)$ is a pulse-like function given by $E(x - L/8 \cdot (x - L/2))E(L/8 \cdot (x - L/2) - x)$. The stability of IMP1 and IMP2 is much higher than EUL and RK2. In Figs. 7 and 8, the accuracy is compared among EUL (Central), EUL (Upwind), IMP1 (Central) and IMP1 (Upwind). The accuracy of IMP1 is very high. In Fig. 9, the accuracy is compared between IMP1 and IMP2. The accuracy of IMP2 is higher than that of IMP1.

5.2. Burgers' equation

The initial-boundary value problem of Burgers' equation is defined by

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = v \frac{\partial^2 u}{\partial x^2} \text{ in } -\infty < x < \infty, \quad (101)$$

$$u(x, 0) = f(x); \quad u(\pm\infty, t) = 0. \quad (102a, b)$$

In the numerical calculation, we replace the infinite region $-\infty < x < \infty$ with a computational region $-L < x < L$. We divide the computational region into N elements $x_i < x < x_{i+1}$, where

$$dx = \frac{2L}{N}; \quad x_i = -L + idx, \quad i = 0, 1, \dots, N. \quad (103a, b)$$

We use the difference operations to approximate the spatial derivatives. If we denote $u(x_i, t)$ as $u_i(t)$, then, we have

$$\frac{du_i}{dt} = -u_i \frac{1}{2dx}(u_{i+1} - u_{i-1}) + v \frac{1}{dx^2}(u_{i+1} - 2u_i + u_{i-1}), \quad i = 0, 1, \dots, N, \quad (104)$$

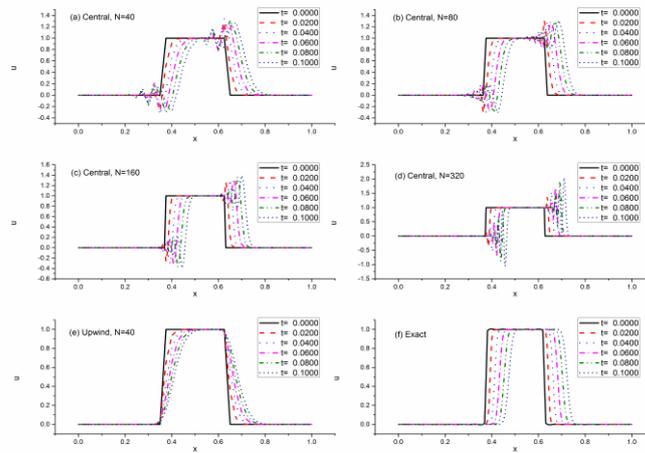


Figure 7: Comparison of accuracy of the solutions by EUL ($f(x)$ ="pulse-like", $V = 1$, $L = 1$, $dt = 0.0025$, $t = 0.1$, $\nu = 0.00089$)

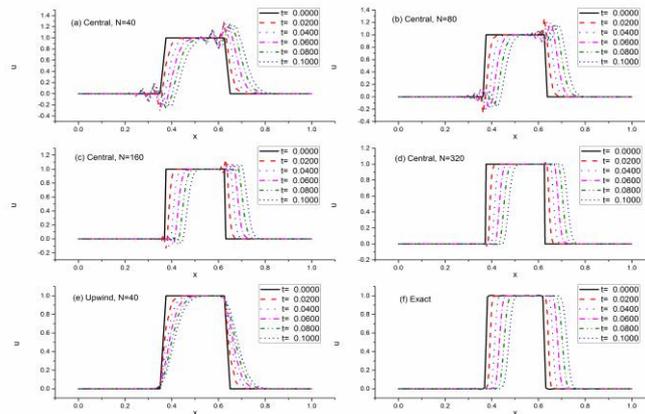


Figure 8: Comparison of accuracy of the solutions by IMP1 ($f(x)$ ="pulse", $V = 1$, $L = 1$, $dt = 0.0025$, $t = 0.1$, $\nu = 0.00089$)

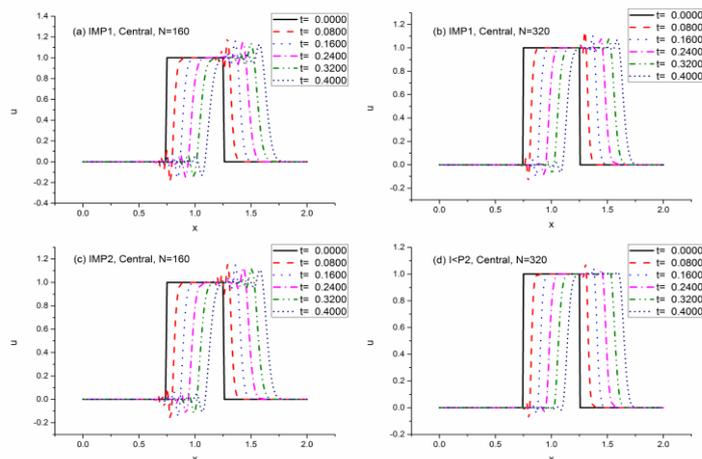


Figure 9: Comparison of accuracy of the solutions between IMP1 and IMP2 ($f(x)$ ="pulse", $V = 1$, $L = 2$, $dt = 0.01$, $t = 0.4$, $\nu = 0.00089$)

$$u_i(0) = f(x_i); \quad u_{-1}(t) = 0, \quad u_{N+1}(t) = 0. \quad (105a, b)$$

Equations (77) and (78) can be rewritten as

$$\left\{ \frac{du}{dt} \right\} = -\frac{1}{dx} \{\phi\} + \frac{\nu}{dx^2} [a] \{u\}, \quad \phi_i = u_i(u_{i+1} - u_{i-1})/2, \quad (106a, b)$$

where

$$\{u\} = [u_0 \quad u_1 \quad \dots \quad u_N]^T, \quad \{\phi\} = [\phi_0 \quad \phi_1 \quad \dots \quad \phi_N]^T, \quad (107, 108)$$

$$a_{0j} = \begin{cases} -2 & \text{for } j=0 \\ 1 & \text{for } j=1 \\ 0 & \text{otherwise} \end{cases}, \quad a_{ij} = \begin{cases} 1 & \text{for } j=i-1 \text{ \& } i+1 \\ -2 & \text{for } j=i \\ 0 & \text{otherwise} \end{cases} \quad \text{for } i=1,2,\dots,N-1, \quad a_{Nj} = \begin{cases} 1 & \text{for } j=N-1 \\ -2 & \text{for } j=N \\ 0 & \text{otherwise} \end{cases}. \quad (109a, b, c)$$

The boundary condition is included in $[a]$.

From Eq. (94), the following time-progressive equations for Euler method (EUL), Implicit method using linear approximation (IMP1), Runge-Kutta method of the 2nd order (RK2) and Implicit method using parabolic approximation (IMP2) are given below, where u_i and ϕ_i at time step n are denoted as $u_i^{(n)}$ and $\phi_i^{(n)}$, respectively. $\phi_i^{(n)}$ is given by

$$\phi_i^{(n)} = u_i^{(n)}(u_{i+1}^{(n)} - u_{i-1}^{(n)})/2. \quad (110)$$

EUL:

$$\{u^{(n+1)}\} = [I] \{u^{(n)}\} - \frac{dt}{dx} \{\phi^{(n)}\} + \frac{\nu dt}{dx^2} [a] \{u^{(n)}\}. \quad (111)$$

IMP1:

$$\{u^{(n+1)}\} = \{u^{(n)}\} - \frac{dt}{dx} \frac{1}{2} \{\phi^{(n)} + \phi^{(n+1)}\} + \frac{\nu dt}{dx^2} [a] \frac{1}{2} \{u^{(n)} + u^{(n+1)}\}, \quad (112a)$$

or

$$\left[I - \frac{\nu dt}{2dx^2} a \right] \{u^{(n+1)}\} = \left[I + \frac{\nu dt}{2dx^2} \right] \{u^{(n)}\} - \frac{dt}{2dx} \{\phi^{(n)}\} - \frac{dt}{2dx} \{\phi^{(n+1)}\}. \quad (112b)$$

RK2:

$$\{u^{(n+1)}\} = \{u^{(n)}\} - \frac{dt}{dx} \{\phi^{(n+1/2)}\} + \frac{\nu dt}{dx^2} [a] \{u^{(n+1/2)}\}, \quad \{u^{(n+1/2)}\} = \{u^{(n)}\} - \frac{dt}{2dx} \{\phi^{(n)}\} + \frac{\nu dt}{2dx^2} [a] \{u^{(n)}\}, \quad (113a, b)$$

$$\phi_i^{(n+1/2)} = u_i^{(n+1/2)}(u_{i+1}^{(n+1/2)} - u_{i-1}^{(n+1/2)})/2. \quad (113c)$$

IMP2

$$\{u^{(n+1/2)}\} = \frac{3}{4} \{u^{(n)}\} - \frac{dt}{dx} \frac{1}{4} \{\phi^{(n)}\} + \frac{\nu dt}{dx^2} [a] \frac{1}{4} \{u^{(n)}\} + \frac{1}{4} \{u^{(n+1)}\}, \quad (114a)$$

$$\{u^{(n+1)}\} = \{u^{(n)}\} - \frac{dt}{dx} \frac{1}{6} \{\phi^{(n)} + 4\phi^{(n+1/2)} + \phi^{(n+1)}\} + \frac{\nu dt}{dx^2} [a] \frac{1}{6} \{u^{(n)} + 4u^{(n+1/2)} + u^{(n+1)}\}. \quad (114b)$$

The initial condition is given by

$$u_i^{(0)} = \begin{cases} -\sin(\pi x_i), & \text{if } |x| \leq 1 \\ 0, & \text{otherwise} \end{cases} \quad \text{for } i=0,1,\dots,N. \quad (115)$$

The boundary condition is included in $[a]$. $\{\phi^{(n+1)}\}$ is determined by iteration.

The exact solution of the initial-boundary value problem, Eqs. (101) and (102), is given in Ref. [3].

The numerical results are shown in Tables 4 and 5 and Figs. 10 and 11. In Tables 4 and 5, ν is the kinematic viscosity, and symbols \circ and \times means whether the calculation is conducted normally or diverged, respectively. The stability of IMP1 is much higher than EUL and RK2. In Figs. 10 and 11, the accuracy is compared among EUL, RK2 and IMP1. The accuracy of IMP1 is very high.

Table 4: $N = 100, t_{\max} = 5$

| | EUL | | | RK2 | | | IMP1 | | |
|------------|-------------|--------------|---------------|-------------|--------------|---------------|-------------|--------------|---------------|
| | $\nu = 0.1$ | $\nu = 0.01$ | $\nu = 0.005$ | $\nu = 0.1$ | $\nu = 0.01$ | $\nu = 0.005$ | $\nu = 0.1$ | $\nu = 0.01$ | $\nu = 0.005$ |
| $dt=0.001$ | \circ | \circ | \times | \circ | \circ | \times | \circ | \circ | \times |
| $dt=0.01$ | \times | \circ | \times | \times | \circ | \times | \circ | \circ | \times |
| $dt=0.1$ | \times | \times | \times | \times | \times | \times | \circ | \circ | \times |

Table 5: $N = 200$, $t_{\max} = 5$

| | EUL | | | RK2 | | | IMP1 | | |
|------------|-------------|--------------|---------------|-------------|--------------|---------------|-------------|--------------|---------------|
| | $\nu = 0.1$ | $\nu = 0.01$ | $\nu = 0.005$ | $\nu = 0.1$ | $\nu = 0.01$ | $\nu = 0.005$ | $\nu = 0.1$ | $\nu = 0.01$ | $\nu = 0.005$ |
| $dt=0.001$ | ○ | ○ | ○ | ○ | ○ | ○ | ○ | ○ | ○ |
| $dt=0.01$ | × | ○ | ○ | × | ○ | × | ○ | ○ | ○ |
| $dt=0.1$ | × | × | × | × | × | × | ○ | ○ | × |

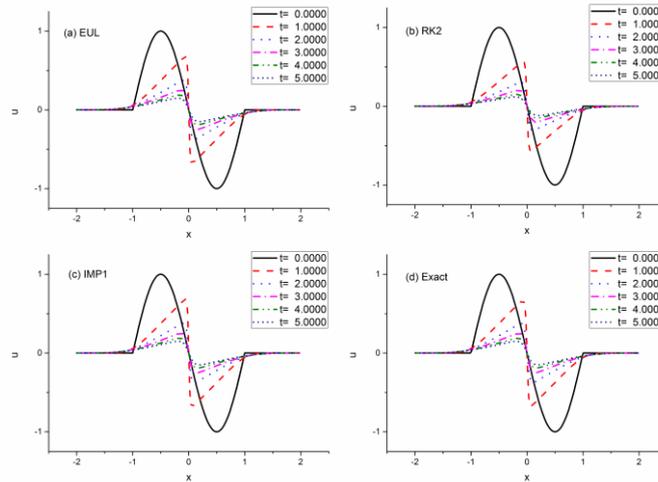


Figure 10: Comparison of accuracy ($N = 200$, $L = 2$, $dt = 0.01$, $\nu = 0.01$)

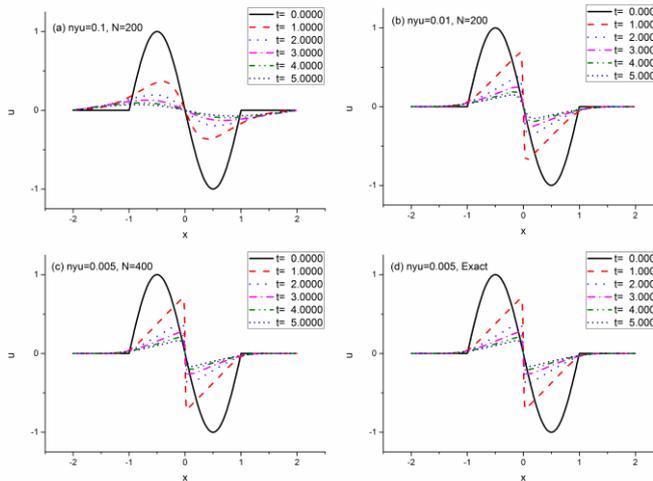


Figure 11: Effects of N and ν on the accuracy (IMP1, $L = 2$, $dt = 0.001$).

5.3. Wave equation

Let x and t be one-dimensional space coordinate and time, and $\phi(x,t)$ be a solution of a initial and boundary value problem of a wave equation:

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{1}{c^2} \frac{\partial^2 \phi}{\partial x^2} = 0 \text{ in } -\infty < x < \infty, \quad (116)$$

$$\phi(x,0) = f(x), \quad \phi_t(x,0) = 0; \quad \phi(\pm\infty, t) = 0, \quad (117a, b)$$

where c is the velocity of wave.

We approximate $-\infty < x < \infty$ by $-L < x < L$ and the discretization of the space is given by Eq. (103). If we denote $\phi(x_i, t)$ as $\phi_i(t)$, then, Eqs. (116) and (117) is approximated for $i = 0, 1, \dots, N$ as

$$\frac{d^2\phi_i}{dt^2} = \frac{1}{dx^2}(\phi_{i+1} - 2\phi_i + \phi_{i-1}), \quad (118)$$

$$\phi_i(0) = f(x_i), \quad \frac{d\phi_i}{dt}(0) = 0; \quad \phi_{-1}(t) = 0, \quad \phi_{N+1}(t) = 0. \quad (119a, b)$$

Equations (118) and (119) can be rewritten for $i = 0, 1, \dots, N$ as

$$\frac{d\phi_i}{dt} = \psi_i, \quad \frac{d\psi_i}{dt} = \frac{1}{dx^2}(\phi_{i+1} - 2\phi_i + \phi_{i-1}), \quad (120a, b)$$

$$\phi_i(0) = f(x_i), \quad \psi_i(0) = 0; \quad \phi_{-1}(t) = 0, \quad \phi_{N+1}(t) = 0. \quad (121a, b)$$

Equation (107) is further rewritten as

$$\left\{ \frac{d\phi}{dt} \right\} = \{\psi\}, \quad \left\{ \frac{d\psi}{dt} \right\} = \frac{1}{dx^2}[a]\{\phi\}, \quad (122a, b)$$

where

$$\{\phi\} = [\phi_0 \quad \phi_1 \quad \dots \quad \phi_N]^T, \quad \{\psi\} = [\psi_0 \quad \psi_1 \quad \dots \quad \psi_N]^T, \quad (123a, b)$$

and $[a]$ is defined by Eq. (109). The boundary condition is included in $[a]$.

From Eq. (122), the following time-progressive equations for Euler method (EUL), Implicit method using linear approximation (IMP1), Runge-Kutta method of the 2nd order (RK2), Implicit method using parabolic approximation (IMP2) and Implicit method using cubic approximation (IMP3) are given below, where ϕ_i and ψ_i at time step n are denoted as $\phi_i^{(n)}$ and $\psi_i^{(n)}$, respectively.

EUL:

$$\{\phi^{(n+1)}\} = \{\phi^{(n)}\} + dt\{\psi^{(n)}\}, \quad \{\psi^{(n+1)}\} = \{\psi^{(n)}\} + \frac{dt}{dx^2}[a]\{\phi^{(n)}\}. \quad (124a, b)$$

IMP1:

$$\{\phi^{(n+1)}\} = \{\phi^{(n)}\} + \frac{dt}{2}\{\psi^{(n+1)} + \psi^{(n)}\}, \quad \{\psi^{(n+1)}\} = \{\psi^{(n)}\} + \frac{dt}{2dx^2}[a]\{\phi^{(n+1)} + \phi^{(n)}\}. \quad (125a, b)$$

or

$$\begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \begin{Bmatrix} \phi^{(n+1)} \\ \psi^{(n+1)} \end{Bmatrix} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix} \begin{Bmatrix} \phi^{(n)} \\ \psi^{(n)} \end{Bmatrix} + \begin{bmatrix} 0 & \frac{dt}{2}I \\ \frac{dt}{2dx^2}a & 0 \end{bmatrix} \begin{Bmatrix} \phi^{(n+1)} + \phi^{(n)} \\ \psi^{(n+1)} + \psi^{(n)} \end{Bmatrix} \quad (126)$$

or

$$\begin{bmatrix} I & -0.5dt \cdot I \\ -0.5\frac{dt}{dx^2}a & I \end{bmatrix} \begin{Bmatrix} \phi^{(n+1)} \\ \psi^{(n+1)} \end{Bmatrix} = \begin{bmatrix} I & 0.5dt \cdot I \\ 0.5\frac{dt}{dx^2}a & I \end{bmatrix} \begin{Bmatrix} \phi^{(n)} \\ \psi^{(n)} \end{Bmatrix}. \quad (127)$$

RK2:

$$t^{(n+1/2)} = t^{(n)} + \frac{dt}{2}, \quad (128a)$$

$$\{\phi^{(n+1/2)}\} = \{\phi^{(n)}\} + \frac{dt}{2}\{\psi^{(n)}\}, \quad \{\psi^{(n+1/2)}\} = \{\psi^{(n)}\} + \frac{dt}{2dx^2}[a]\{\phi^{(n)}\}, \quad (128b, c)$$

$$\{\phi^{(n+1)}\} = \{\phi^{(n)}\} + dt\{\psi^{(n+1/2)}\}, \quad \{\psi^{(n+1)}\} = \{\psi^{(n)}\} + dt\frac{1}{dx^2}[a]\{\phi^{(n+1/2)}\}, \quad (128d, e)$$

IMP2:

$$\{\phi^{(n+1/2)}\} = \frac{3}{4}\{\phi^{(n)}\} + \frac{dt}{4}\{\psi^{(n)}\} + \frac{1}{4}\{\phi^{(n+1)}\}, \quad \{\psi^{(n+1/2)}\} = \frac{3}{4}\{\psi^{(n)}\} + \frac{dt}{4dx^2}[a]\{\phi^{(n)}\} + \frac{1}{4}\{\psi^{(n+1)}\}, \quad (129a, b)$$

$$\{\phi^{(n+1)}\} = \{\phi^{(n)}\} + \frac{dt}{6}\{\psi^{(n)} + 4\psi^{(n+1/2)} + \psi^{(n+1)}\}, \quad \{\psi^{(n+1)}\} = \{\psi^{(n)}\} + \frac{dt}{6dx^2}[a]\{\phi^{(n)} + 4\phi^{(n+1/2)} + \phi^{(n+1)}\} \quad (129c, d)$$

or

$$\begin{Bmatrix} \phi^{(n+1/2)} \\ \psi^{(n+1/2)} \end{Bmatrix} = \begin{bmatrix} \frac{3}{4}I & \frac{dt}{4}I \\ \frac{dt}{4dx^2}a & \frac{3}{4}I \end{bmatrix} \begin{Bmatrix} \phi^{(n)} \\ \psi^{(n)} \end{Bmatrix} + \frac{1}{4} \begin{Bmatrix} \phi^{(n+1)} \\ \psi^{(n+1)} \end{Bmatrix}, \quad (130a)$$

$$\begin{Bmatrix} \phi^{(n+1)} \\ \psi^{(n+1)} \end{Bmatrix} = \begin{bmatrix} I & \frac{dt}{6} I \\ \frac{dt}{6dx^2} a & I \end{bmatrix} \begin{Bmatrix} \phi^{(n)} \\ \psi^{(n)} \end{Bmatrix} + \begin{bmatrix} 0 & \frac{4dt}{6} I \\ \frac{4dt}{6dx^2} a & 0 \end{bmatrix} \begin{Bmatrix} \phi^{(n+1/2)} \\ \psi^{(n+1/2)} \end{Bmatrix} + \begin{bmatrix} 0 & \frac{dt}{6} I \\ \frac{dt}{6dx^2} a & 0 \end{bmatrix} \begin{Bmatrix} \phi^{(n+1)} \\ \psi^{(n+1)} \end{Bmatrix}. \quad (130b)$$

Substituting Eq. (130b) into Eq. (130a)

$$\begin{bmatrix} I & -\frac{dt}{3} I \\ -\frac{dt}{3dx^2} a & I \end{bmatrix} \begin{Bmatrix} \phi^{(n+1)} \\ \psi^{(n+1)} \end{Bmatrix} = \begin{bmatrix} I + \frac{dt^2}{6dx^2} a & \frac{2dt}{3} I \\ \frac{2dt}{3dx^2} a & I + \frac{dt^2}{6dx^2} a \end{bmatrix} \begin{Bmatrix} \phi^{(n)} \\ \psi^{(n)} \end{Bmatrix}. \quad (131)$$

IMP3

$$\{f_\phi^{(n)}\} = \{\psi^{(n)}\}, \{f_\phi^{(n+1/3)}\} = \{\psi^{(n+1/3)}\}, \{f_\phi^{(n+2/3)}\} = \{\psi^{(n+2/3)}\}, \{f_\phi^{(n+1)}\} = \{\psi^{(n+1)}\}, \quad (132a, b, c, d)$$

$$\{f_\psi^{(n)}\} = \frac{1}{dx^2} [a] \{\phi^{(n)}\}, \{f_\psi^{(n+1/3)}\} = \frac{1}{dx^2} [a] \{\phi^{(n+1/3)}\}, \{f_\psi^{(n+2/3)}\} = \frac{1}{dx^2} [a] \{\phi^{(n+2/3)}\}, \{f_\psi^{(n+1)}\} = \frac{1}{dx^2} [a] \{\phi^{(n+1)}\}, \quad (132e, f, g, h)$$

$$\{p_\phi^{(n)}\} = \frac{1}{dt^2} \{3\phi^{(n+1)} - 3\phi^{(n)} - 2f_\phi^{(n)} dt - f_\phi^{(n+1)} dt\}, \{q_\phi^{(n)}\} = -\frac{1}{dt^3} \{2\phi^{(n+1)} - 2\phi^{(n)} - f_\phi^{(n)} dt - f_\phi^{(n+1)} dt\}, \quad (132i, j)$$

$$\{\phi^{(n+1/3)}\} = \left\{ \phi^{(n)} + f_\phi^{(n)} \frac{dt}{3} + p_\phi^{(n)} \frac{dt^2}{9} + q_\phi^{(n)} \frac{dt^3}{27} \right\}, \{\phi^{(n+2/3)}\} = \left\{ \phi^{(n)} + f_\phi^{(n)} \frac{2dt}{3} + p_\phi^{(n)} \frac{4dt^2}{9} + q_\phi^{(n)} \frac{8dt^3}{27} \right\}, \quad (132k, l)$$

$$\{p_\psi^{(n)}\} = \frac{1}{dx^2} \{3\psi^{(n+1)} - 3\psi^{(n)} - 2f_\psi^{(n)} dt - f_\psi^{(n+1)} dt\}, \{q_\psi^{(n)}\} = -\frac{1}{dx^3} \{2\psi^{(n+1)} - 2\psi^{(n)} - f_\psi^{(n)} dt - f_\psi^{(n+1)} dt\}, \quad (132m, n)$$

$$\{\psi^{(n+1/3)}\} = \left\{ \psi^{(n)} + f_\psi^{(n)} \frac{dt}{3} + p_\psi^{(n)} \frac{dt^2}{9} + q_\psi^{(n)} \frac{dt^3}{27} \right\}, \{\psi^{(n+2/3)}\} = \left\{ \psi^{(n)} + f_\psi^{(n)} \frac{2dt}{3} + p_\psi^{(n)} \frac{4dt^2}{9} + q_\psi^{(n)} \frac{8dt^3}{27} \right\}, \quad (132o, p)$$

$$I(a, b, m_1, m_2, m_3) = \left[\frac{1}{4} (b^4 - a^4) - \frac{1}{3} (m_1 + m_2 + m_3) (b^3 - a^3) + \frac{1}{2} (m_1 m_2 + m_2 m_3 + m_3 m_1) (b^2 - a^2) - m_1 m_2 m_3 (b - a) \right], \quad (132q)$$

$$F_{n,0} = \frac{I(t_n, t_{n+1}, t_{n+1/3}, t_{n+2/3}, t_{n+1})}{(t_n - t_{n+1/3})(t_n - t_{n+2/3})(t_n - t_{n+1})} = -\frac{9}{2dt^3} I(t_n, t_{n+1}, t_{n+1/3}, t_{n+2/3}, t_{n+1}), \quad (132r)$$

$$F_{n,1/3} = \frac{I(t_n, t_{n+1}, t_n, t_{n+2/3}, t_{n+1})}{(t_{n+1/3} - t_n)(t_{n+1/3} - t_{n+2/3})(t_{n+1/3} - t_{n+1})} = \frac{27}{2dt^3} I(t_n, t_{n+1}, t_n, t_{n+2/3}, t_{n+1}), \quad (132s)$$

$$F_{n,2/3} = \frac{I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+1})}{(t_{n+2/3} - t_n)(t_{n+2/3} - t_{n+1/3})(t_{n+2/3} - t_{n+1})} = -\frac{27}{2dt^3} I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+1}), \quad (132t)$$

$$F_{n,1} = \frac{I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+2/3})}{(t_{n+1} - t_n)(t_{n+1} - t_{n+1/3})(t_{n+1} - t_{n+2/3})} = \frac{9}{2dt^3} I(t_n, t_{n+1}, t_n, t_{n+1/3}, t_{n+2/3}), \quad (132u)$$

$$\{\phi^{(n+1)}\} = \{\phi^{(n)}\} + \{F^{(n)} f_\phi^{(n)} + F^{(n+1/3)} f_\phi^{(n+1/3)} + F^{(n+2/3)} f_\phi^{(n+2/3)} + F^{(n+1)} f_\phi^{(n+1)}\}, \quad (132v)$$

$$\{\psi^{(n+1)}\} = \{\psi^{(n)}\} + \{F^{(n)} f_\psi^{(n)} + F^{(n+1/3)} f_\psi^{(n+1/3)} + F^{(n+2/3)} f_\psi^{(n+2/3)} + F^{(n+1)} f_\psi^{(n+1)}\}. \quad (132w)$$

The initial condition is given by

$$f_i^{(0)} = \exp \left[-\left(\frac{x_i}{L/10} \right)^2 \right] \text{ for } i = 0, 1, \dots, N. \quad (133)$$

The boundary condition is included in $[a]$. $\{\phi^{(n+1)}\}$ and $\{\psi^{(n+1)}\}$ are determined by iteration.

The exact solution of the initial-boundary value problem, Eqs. (116) and (117), is given by

$$\phi(x, t) = f(x - ct), \quad \psi(x, t) = \partial \phi / \partial t = -cf'(x - ct). \quad (134a, b)$$

The numerical results are shown in Figs. 12-18. According to the results in Figs. 12-17, the stability and accuracy of IMP1 is much higher than EUL and RK2 in case of a bell-shape initial value. In Fig. 18, IMP1, IMP2 and IMP3 are compared in case of a triangular initial value. Although the accuracy was higher in the order of IMP1, IMP2 and IMP3, large difference was not observed among the three solutions.

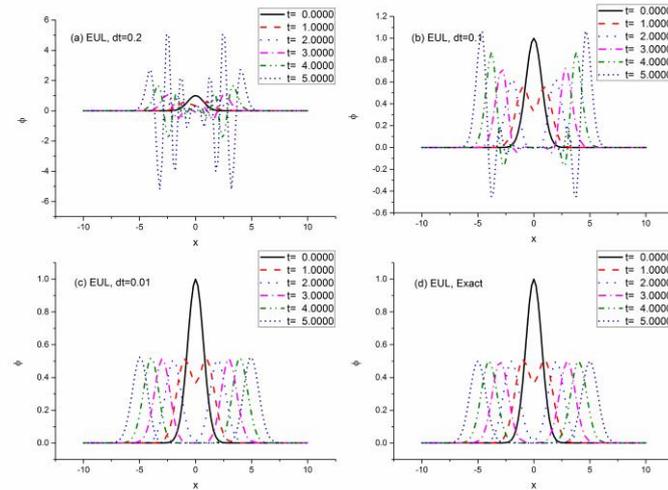


Figure 12: ϕ , EUL, $L=10$, $N=100$, $t_{max}=5$

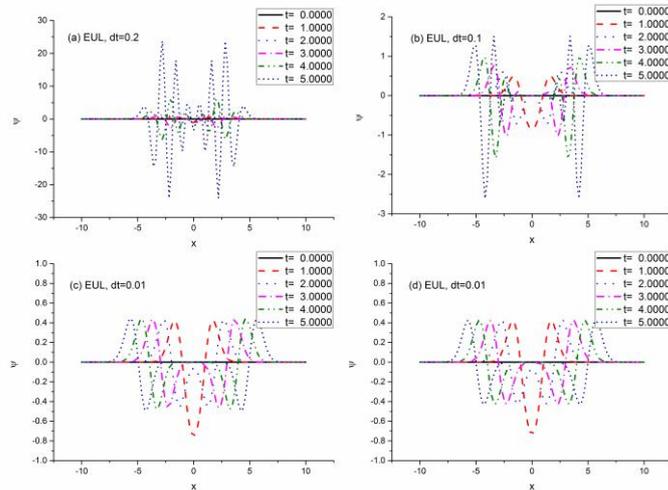


Figure 13: ψ , EUL, $L=10$, $N=100$, $t_{max}=5$

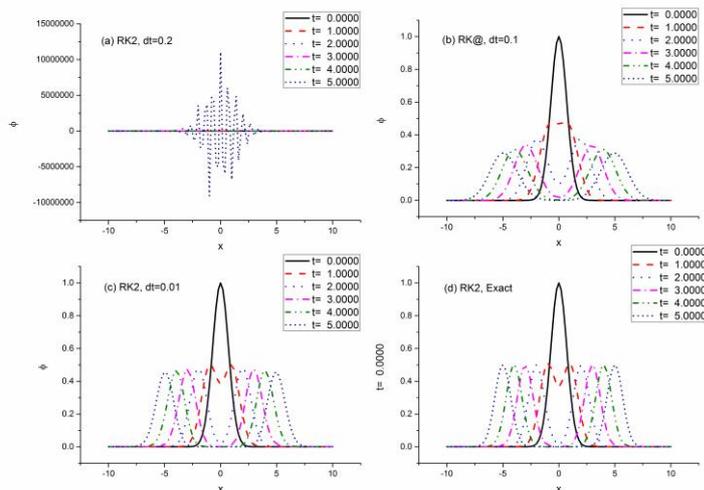


Figure 14: ϕ , RK2, $L=10$, $N=100$, $t_{max}=5$

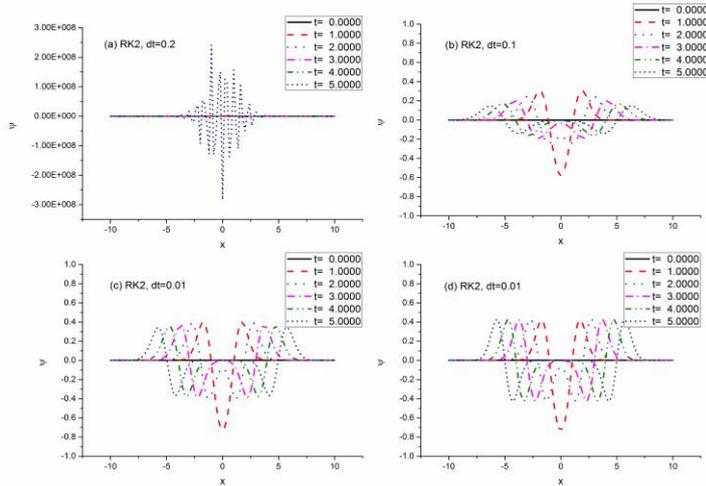


Figure 15: ψ , RK2, $L=10$, $N=100$, $t_{\max}=5$

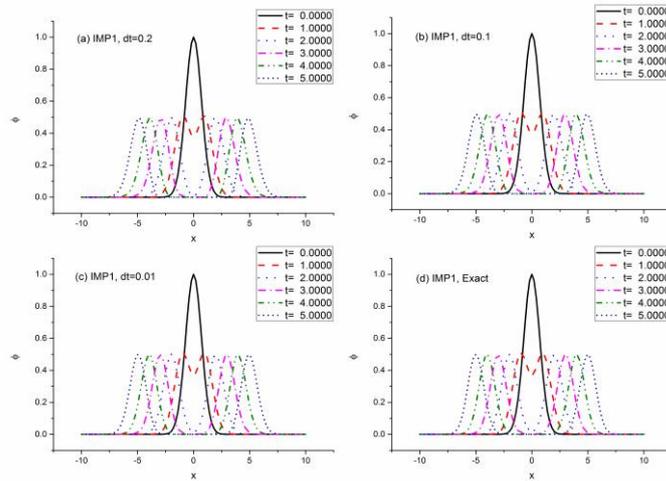


Figure 16: ϕ , IMP1, $L=10$, $N=100$, $t_{\max}=5$

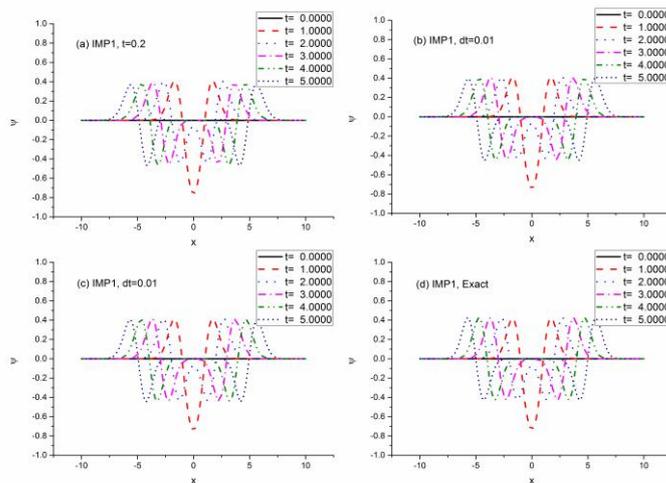


Figure 17: ψ , IMP1, $L=10$, $N=100$, $t_{\max}=5$

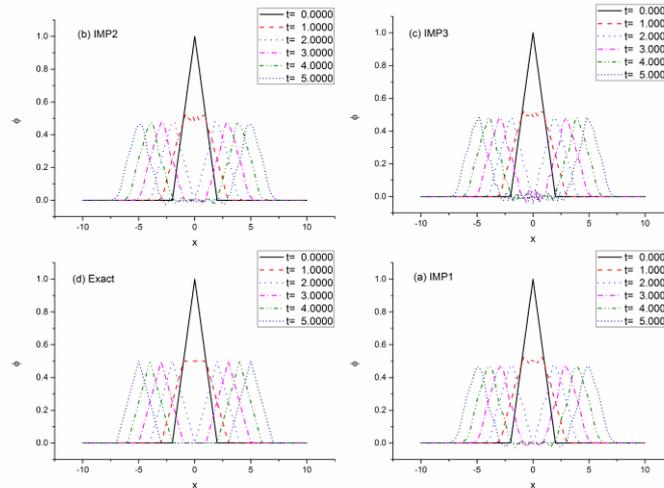


Figure 18: Comparison of IMP1, IMP2 and IMP3 of ϕ , $L = 10$, $N = 100$, $dt = 0.1$, $t_{\max} = 5$

6. CONCLUSIONS

The stability and accuracy of the numerical integration of the time-evolution equation has a crucial importance in solving the unsteady partial differential equation. Crank-Nicolson [1] and Rosenbrock [2] have discussed not only the stability but also the accuracy theoretically. In the present paper, the same problems were discussed again from the different viewpoint and verified by the numerical results.

The Runge-Kutta methods are widely used in the numerical integration. However, in some cases, the stability is not sufficient. In these cases, the implicit method is effective in increasing the stability.

New implicit methods were proposed to increase stability and accuracy of the solution of the time-evolution equation. The stability of various methods including Runge-Kutta method was discussed theoretically and numerically, and the numerical examples were shown to show the effectiveness of the New Implicit methods.

As implicit methods, we proposed implicit method using linear approximation (IMP1), one using parabolic approximation (IMP2) and one using cubic approximation (IMP3). In the case of linear problem, IMP1 is identical to the implicit method by Crank and Nicholson [1]. However, the algorithms of the higher approximation become difficult, although the implicit methods increase the stability drastically. Of course, the accuracy is also increased. Since, the accuracy is increased by using finer spatial mesh, the most practical way to increase the accuracy and the stability in the solution of unsteady boundary value problems may be to use IMP1 and the smaller spatial mesh size.

The effects of nonlinearity on the implicit methods were also discussed. Unsteady Burgers' equation was solved numerically using the Euler Methods, RK2 and IMP1. IMP1 gave the best results both in accuracy and stability.

7. REFERENCES

The author express sincere gratitude to Prof. S. Nagata and Prof. Y. Imai of Saga University, Japan for their continuous cooperation.

8. REFERENCES

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APPENDIX A. STABILITY ANALYSIS BY CRANK-NICHOLSON'S METHOD [1]

We study the stability of the problem discussed in Section 2.1.2 according to a method by Crank and Nicholson [1]. The differential equation is given by

$$\frac{du}{dt} = -u + f. \quad (\text{A.1})$$

First, we use Euler method using central difference is used for the numerical integration of Eq. (A.1). Then, the solution u_n at time step $t_n = ndt$ satisfies the following difference equation:

$$u_{n+1} - u_{n-1} = -2dtu_n + dt f_n. \quad (\text{A.2})$$

Let u'_n be a solution of Eq. (A.2) with the computational error Δu_n , namely

$$u'_n = u_n + \Delta u_n. \quad (\text{A.3})$$

Substituting Eq. (A.3) into Eq. (A.2), we have

$$\Delta u_{n+1} - \Delta u_{n-1} = -2dt \Delta u_n. \quad (\text{A.4})$$

If we assume

$$\Delta u_n = Ae^{kndt}, \quad (\text{A.5})$$

we obtain

$$e^{kdt} - e^{-kdt} = -2dt \text{ or } \sinh(kdt) = -dt. \quad (\text{A.6, 7})$$

Equation (A.7) means $k < 0$, and Δu_n is derived as

$$\Delta u_n = Ae^{kndt} + B(-1)^n e^{-kndt}. \quad (\text{A.8})$$

The first term Ae^{kndt} converges to zero, and the second term $B(-1)^n e^{-kndt}$ alternates sign in successive time steps and increase magnitude exponentially. Hence, the solution of Eq. (A.2) oscillates with increasing amplitude.

If we use Euler method given by the following difference equation:

$$u_{n+1} - u_n = -dtu_n + dt f_n, \quad (\text{A.9})$$

then, we have

$$\Delta u_{n+1} - \Delta u_n = -dt \Delta u_n. \quad (\text{A.10})$$

Substituting Eq. (A.5) into Eq. (A.10), we obtain

$$Ae^{k(n+1)dt} - Ae^{kndt} = -dtAe^{kndt} \text{ or } e^{kdt} = 1 - dt. \quad (\text{A.11, 12})$$

Hence, if $0 < dt < 1$, $\Delta u_n = Ae^{kndt}$ converges to zero. However, if $dt > 1$, then, k becomes complex: $e^{kdt} = 1 - dt = -(dt - 1) = e^{\ln(dt-1)+i\pi}$. So, we have

$$\Delta u_n = Ae^{kndt} = Ae^{n(a+i\pi)} = (-1)^n Ae^{na} = (-1)^n A(dt - 1)^n. \quad (\text{A.13})$$

Hence, if $1 < dt < 2$ or $2 < dt$, then, Δu_n converges to zero or diverges to infinity alternating sign in successive time steps, respectively.

If we use implicit method, the difference equation is given by

$$u_{n+1} - u_n = -\frac{1}{2}dt(u_n + u_{n+1}) + \frac{1}{2}f(n + 0.5dt). \quad (\text{A.14})$$

or

$$\left(1 + \frac{1}{2}dt\right)u_{n+1} = \left(1 - \frac{1}{2}dt\right)u_n + \frac{1}{2}f(n + 0.5dt). \quad (\text{A.15})$$

Substituting Eq. (A.3) into Eq. (A.15), we have

$$\left(1 + \frac{1}{2}dt\right)\Delta u_{n+1} = \left(1 - \frac{1}{2}dt\right)\Delta u_n. \quad (\text{A.16})$$

Substituting Eq. (A.5) into Eq. (A.16), we obtain

$$\left(1 + \frac{1}{2}dt\right)Ae^{k(n+1)dt} = \left(1 - \frac{1}{2}dt\right)Ae^{kndt} \text{ or } e^{kdt} = \left(1 - \frac{1}{2}dt\right) / \left(1 + \frac{1}{2}dt\right). \quad (\text{A.18})$$

Since $0 < e^{kdt} < 1$, then, $k < 0$, and Δu_n converges always to zero.

APPENDIX B. FORMULAE OF NUMERICAL INTEGRATION OF A CUBIC FUNCTION

Equation (64) is explained below:

$$\begin{aligned}
 & \int_{x_n}^{x_{n+1}} f(x, y(x)) dx \\
 & \approx \int_{x_n}^{x_{n+1}} \left[f_n \frac{(x - x_{n+1/3})(x - x_{n+2/3})(x - x_{n+1})}{(x_n - x_{n+1/3})(x_n - x_{n+2/3})(x_n - x_{n+1})} + f_{n+1/3} \frac{(x - x_n)(x - x_{n+2/3})(x - x_{n+1})}{(x_{n+1/3} - x_n)(x_{n+1/3} - x_{n+2/3})(x_{n+1/3} - x_{n+1})} \right. \\
 & \quad \left. + f_{n+2/3} \frac{(x - x_n)(x - x_{n+1/3})(x - x_{n+1})}{(x_{n+2/3} - x_n)(x_{n+2/3} - x_{n+1/3})(x_{n+2/3} - x_{n+1})} + f_{n+1} \frac{(x - x_n)(x - x_{n+1/3})(x - x_{n+2/3})}{(x_{n+1} - x_n)(x_{n+1} - x_{n+1/3})(x_{n+1} - x_{n+2/3})} \right] dx \\
 & = \left[f_n \frac{I(x_n, x_{n+1}, x_{n+1/3}, x_{n+2/3}, x_{n+1})}{(x_n - x_{n+1/3})(x_n - x_{n+2/3})(x_n - x_{n+1})} + f_{n+1/3} \frac{I(x_n, x_{n+1}, x_n, x_{n+2/3}, x_{n+1})}{(x_{n+1/3} - x_n)(x_{n+1/3} - x_{n+2/3})(x_{n+1/3} - x_{n+1})} \right. \\
 & \quad \left. + f_{n+2/3} \frac{I(x_n, x_{n+1}, x_n, x_{n+1/3}, x_{n+1})}{(x_{n+2/3} - x_n)(x_{n+2/3} - x_{n+1/3})(x_{n+2/3} - x_{n+1})} + f_{n+1} \frac{I(x_n, x_{n+1}, x_n, x_{n+1/3}, x_{n+2/3})}{(x_{n+1} - x_n)(x_{n+1} - x_{n+1/3})(x_{n+1} - x_{n+2/3})} \right]. \tag{B.1}
 \end{aligned}$$

where

$$\begin{aligned}
 I(a, b, m_1, m_2, m_3) &= \int_a^b (x - m_1)(x - m_2)(x - m_3) dx \\
 &= \int_a^b [x^3 - (m_1 + m_2 + m_3)x^2 + (m_1m_2 + m_2m_3 + m_3m_1)x - m_1m_2m_3] dx \\
 &= \left[\frac{1}{4}x^4 - \frac{1}{3}(m_1 + m_2 + m_3)x^3 + \frac{1}{2}(m_1m_2 + m_2m_3 + m_3m_1)x^2 - m_1m_2m_3x \right]_{x=a}^{x=b} \\
 &= \frac{1}{4}(b^4 - a^4) - \frac{1}{3}(m_1 + m_2 + m_3)(b^3 - a^3) + \frac{1}{2}(m_1m_2 + m_2m_3 + m_3m_1)(b^2 - a^2) - m_1m_2m_3(b - a). \tag{B.2}
 \end{aligned}$$