

MECH5230 Homework Assignment

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1 1D Time-dependent Heat Equation

Solve the time-dependent heat equation $T_t = \alpha T_{xx}$, $0 \leq x \leq L$.

Initial condition: $T(x, 0) = c \sin(\pi x/L)$.

Boundary condition: $T(0, t) = T(L, t) = 0$.

Exact solution is $T_{exact}(x, t) = c \exp(-\alpha \pi^2 t/L^2) \sin(\pi x/L)$

Let $c = 100^\circ C$, $L = 1m$, $\alpha = 0.02m^2/h$.

1. Simple explicit method.

Forward Time Central Space (FTCS):

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2} \quad (1)$$

i.e.,

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n) \quad (2)$$

2. Alternating direction explicit (ADE) method proposed by Barakat and Clark.

the calculation procedure is simultaneously marched in both directions (p_i^{n+1} is updated from left-side points, while q_i^{n+1} is updated from right-side points) the resulting solution are averaged to obtain the final value of T_i^{n+1} .

$$\begin{aligned} \frac{p_i^{n+1} - p_i^n}{\Delta t} &= \alpha \frac{p_{i+1}^n - p_i^n - p_i^{n+1} + p_{i-1}^{n+1}}{(\Delta x)^2} \\ \frac{q_i^{n+1} - q_i^n}{\Delta t} &= \alpha \frac{q_{i+1}^{n+1} - q_i^{n+1} - q_i^n + q_{i-1}^n}{(\Delta x)^2} \\ T_i^{n+1} &= \frac{1}{2} (p_i^{n+1} + q_i^{n+1}) \end{aligned} \quad (3)$$

i.e.,

$$\begin{aligned} p_i^{n+1} [1 + \frac{\alpha \Delta t}{(\Delta x)^2}] &= \frac{\alpha \Delta t}{(\Delta x)^2} p_{i-1}^{n+1} + [1 - \frac{\alpha \Delta t}{(\Delta x)^2}] p_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} p_{i+1}^n \\ q_i^{n+1} [1 + \frac{\alpha \Delta t}{(\Delta x)^2}] &= \frac{\alpha \Delta t}{(\Delta x)^2} q_{i+1}^{n+1} + [1 - \frac{\alpha \Delta t}{(\Delta x)^2}] q_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} q_{i-1}^n \\ T_i^{n+1} &= \frac{1}{2} (p_i^{n+1} + q_i^{n+1}) \end{aligned} \quad (4)$$

1.1 Comparison of FTCS and ADE Scheme

For $\Delta x = 0.1$ and $\Delta t = 0.1$ compare results for $t = 10h$ in a graph, as shown in Fig.1(a)

1.2 Accuracy of FTCS Scheme

Refining the mesh as $\Delta x = 0.066667$ while remaining the time step as $\Delta t = 0.1h$ compare results for $t = 10h$ in a graph, as shown in Fig.1(b)

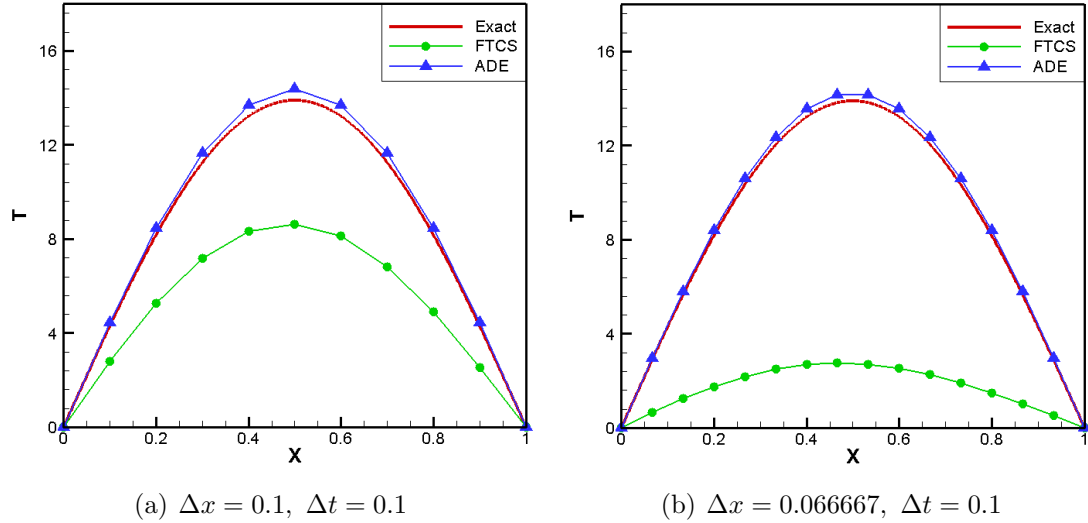


Figure 1: Comparison results of FTCS (Forward Time Central Space) and ADE (Alternating Direction Explicit) scheme ($t = 10h$) with different mesh resolution

For FTCS scheme, after refining the mesh, however, the error does **NOT** reduce as suggested by $O(\Delta x^2)$. This is mainly due to the reason that for FTCS scheme, the error is related with both space step and time step, i.e., $O(\Delta x^2, \Delta t)$. The influence of time step Δt on error is prominent for time-dependent problem. Later we will found different situation in Problem 2(2), where a steady problem is considered.

1.3 Stability of FTCS Scheme

For FTCS scheme, the error is $O(\Delta x^2, \Delta t)$. At given mesh resolution (Δx), the error will be dependent on Δt .

Define CFL number as

$$CFL = \frac{\alpha \Delta t}{(\Delta x)^2} \quad (5)$$

by choose smaller Δt (i.e., choose smaller CFL number), we can actually reduce the error.

Here, we choose $\Delta x = 0.1$ and $CFL = 0.06, 0.6$.

Define L^2 norm error of temperature as

$$Error(t) = \sqrt{\frac{\sum [T_{numerical}(t) - T_{exact}(t)]^2}{\sum T_{exact}(t)^2}} \quad (6)$$

We can found from Fig.2 that L^2 norm error of temperature for $CFL = 0.6$ progressively become larger, while slightly change for $CFL = 0.06$.

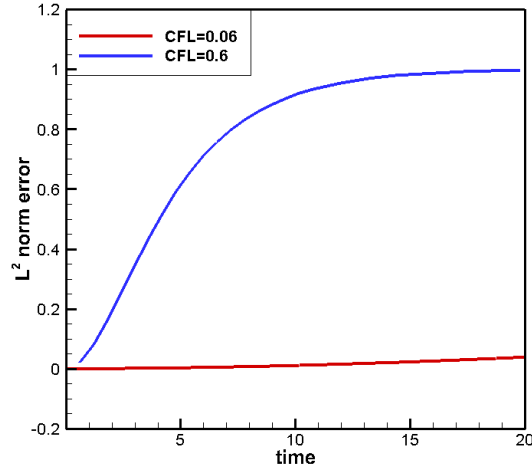


Figure 2: Error evolution within 20h of problem time under different CFL number for FTCS method

1.4 Accuracy of ADE Scheme

Again, define CFL number as

$$CFL = \frac{\alpha \Delta t}{(\Delta x)^2} \quad (7)$$

Choose $\Delta x = 0.1$ and $CFL = 1, 2, 3$, compare corresponding results with exact solution as shown in Fig.3. We can found, as CFL number increase, the discrepancy becomes noticeable.

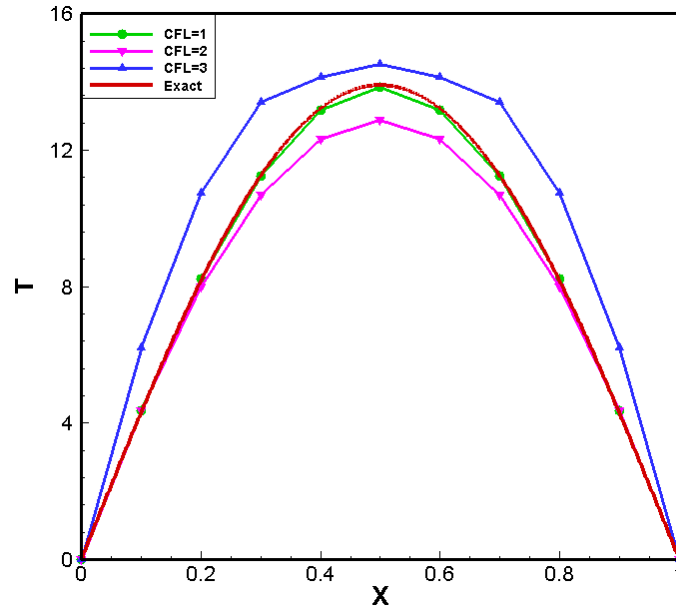


Figure 3: Comparison ADE results of FTCS under different CFL number

2 1D Steady-state Heat Equation with Source Term

Solve heat equation with a source term $T_t = \alpha T_{xx} + S(x)$, $0 \leq x \leq L_x$.

Initial condition: $T(x, 0) = 0$.

Boundary condition: $T(0, t) = 0$, $T(L_x, t) = T_{steady}(L_x)$.

Exact steady solution is $T_{steady}(x) = x^2 e^{-x}$.

Let $\alpha = 1$, $L_x = 15$, $S(x) = -(x^2 - 4x + 2)e^{-x}$.

2.1 Exact Solution

Verify the exact steady solution is $T_{steady}(x) = x^2 e^{-x}$.

For steady solution, $T_t = 0$, then the heat equation at steady state is

$$\alpha T_{xx} + S(x) = 0 \quad (8)$$

Since,

$$\begin{aligned} S(x) &= -(x^2 - 4x + 2)e^{-x} \\ T(x) &= x^2 e^{-x} \\ T_x(x) &= 2xe^{-x} - x^2 e^{-x} = (2x - x^2)e^{-x} \\ T_{xx}(x) &= (2 - 2x)e^{-x} - (2x - x^2)e^{-x} = (2 - 4x + x^2)e^{-x} \end{aligned} \quad (9)$$

thus,

$$\alpha T_{xx}(x) + S(x) = (2 - 4x + x^2)e^{-x} - (x^2 - 4x + 2)e^{-x} = 0 \quad (10)$$

proving that exact solution is $T_{steady}(x) = x^2e^{-x}$

Plot exact solution as shown in Fig.4.

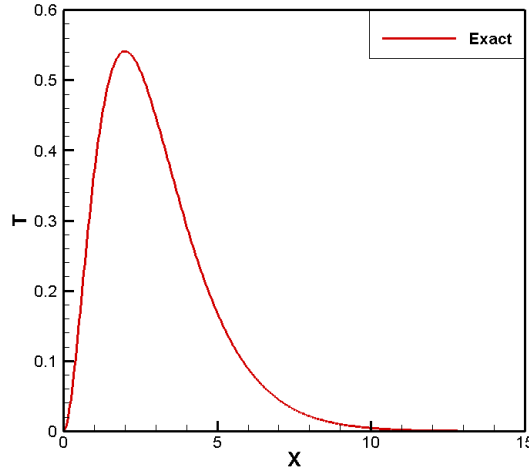


Figure 4: Exact solution of 1D heat equation with source term

2.2 FTCS Scheme

Explicit Euler for time advancement and second-order central difference scheme on a uniform grid:

$$X_i = i \cdot \Delta x \quad (11)$$

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2} + S(X_i) \quad (12)$$

i.e.,

$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{(\Delta x)^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n) - \Delta t (X_i^2 - 4X_i + 2)e^{-X_i} \quad (13)$$

Plot the exact and numerical steady solutions for $N_x = 10, 20$ as Fig.5.

We can found that increase the grid numbers indeed reduce the error. It should be noted that different from Problem 1.(2), which is time-dependent problem, the error is $O(\Delta x^2, \Delta t)$. While for steady problem, like this one, Δt have little influence on the error. Small Δt requires longer iterative steps to converge to steady solution, while larger Δt requires less (so long the program is stable). The influence of space step Δx on error is prominent for steady problem. Thus, refine the mesh resolution reduces the error.

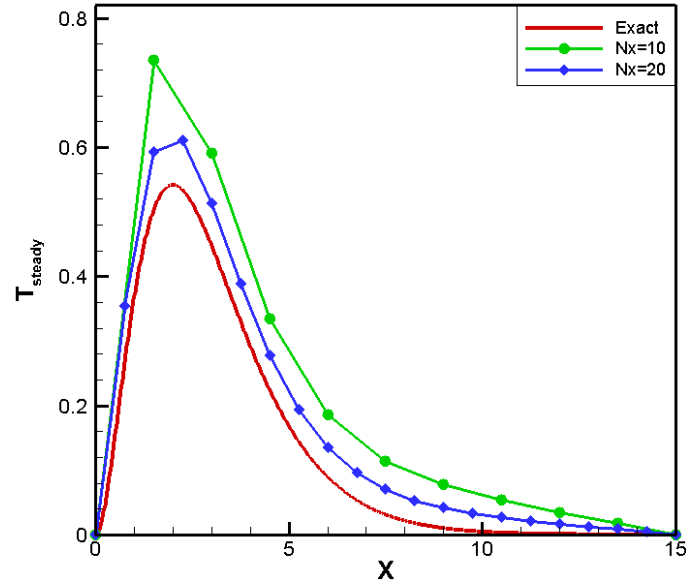


Figure 5: Results of FTCS with different uniform mesh grids

2.3 Non-uniform Grid

On a non-uniform grid $X_j = L_x[1 - \cos(\frac{\pi j}{2N_x})]$, perform Taylor expansion,

$$\begin{aligned} f_{j+1} &= f_j + \Delta x_{j+1} f'_j + \frac{(\Delta x_{j+1})^2}{2} f''_j + \frac{(\Delta x_{j+1})^3}{3!} f'''_j + \dots \\ f_{j-1} &= f_j - \Delta x_j f'_j + \frac{(\Delta x_j)^2}{2} f''_j - \frac{(\Delta x_j)^3}{3!} f'''_j + \dots \end{aligned} \quad (14)$$

thus, we have

$$f''_j = 2 \frac{\Delta x_j (f_{j+1} - f_j) - \Delta x_{j+1} (f_j - f_{j-1})}{\Delta x_j \Delta x_{j+1} (\Delta x_j + \Delta x_{j+1})} \quad (15)$$

where $\Delta x_j = X_j - X_{j-1}$.

Discretization of heat equation leads to

$$\begin{aligned} \frac{T_j^{n+1} - T_j^n}{\Delta t} &= \alpha 2 \frac{\Delta x_j (T_{j+1}^n - T_j^n) - \Delta x_{j+1} (T_j^n - T_{j-1}^n)}{\Delta x_j \Delta x_{j+1} (\Delta x_j + \Delta x_{j+1})} - (X_j^2 - 4X_j + 2)e^{-X_j} \\ X_j &= L_x[1 - \cos(\frac{\pi j}{2N_x})] \\ \Delta x_j &= X_j - X_{j-1} \end{aligned} \quad (16)$$

A comparison of grids is shown in Fig.6

Plot the exact and numerical steady solutions for $N_x = 10, 20$ as Fig.7.

Compare Fig.5 and Fig.7 we can conclude using more (non-uniform grid) points in the region where solution changes rapidly (e.g., $0 \leq x \leq 5$) will reduce the error.



Figure 6: Comparison of non-uniform grid and uniform grid ($N_x = 10$)

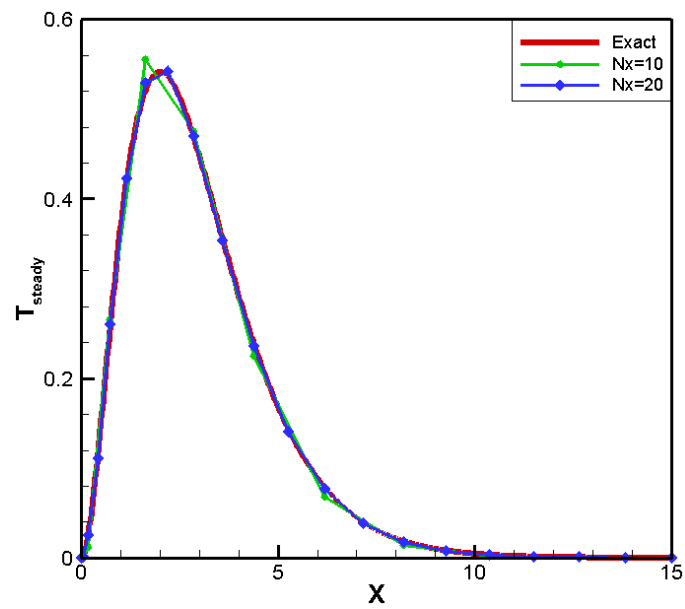


Figure 7: Results of FTCS with different non-uniform mesh grids

2.4 Coordinate Transformation

Transform the differential equation a new coordinate system using the transform $\xi_j = \cos^{-1}(1 - X_j/L_x)$.

$$\begin{aligned} X_j &= L_x[1 - \cos(\frac{\pi j}{2N_x})] \\ \xi_j &= \frac{\pi j}{2N_x} \end{aligned} \quad (17)$$

Based on the chain rule of derivatives, the transformation is conducted as

$$\text{Define : } A = \frac{\partial}{\partial x}, \text{ thus, } A = \left(\frac{\partial \xi}{\partial x}\right) \frac{\partial}{\partial \xi} \quad (18)$$

$$\text{Define : } B = \frac{\partial^2}{\partial x \partial \xi} = \frac{\partial}{\partial x} \left(\frac{\partial}{\partial \xi}\right), \text{ thus, } B = A \left(\frac{\partial}{\partial \xi}\right) = \left(\frac{\partial \xi}{\partial x}\right) \frac{\partial}{\partial \xi} \left(\frac{\partial}{\partial \xi}\right) = \left(\frac{\partial \xi}{\partial x}\right) \left(\frac{\partial^2}{\partial \xi^2}\right) \quad (19)$$

$$\frac{\partial^2}{\partial x^2} = \frac{\partial A}{\partial x} = \frac{\partial}{\partial x} \left(\frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi}\right) = \frac{\partial^2 \xi}{\partial x^2} \frac{\partial}{\partial \xi} + \frac{\partial \xi}{\partial x} \frac{\partial^2}{\partial x \partial \xi} = \left(\frac{\partial^2 \xi}{\partial x^2}\right) \left(\frac{\partial}{\partial \xi}\right) + \left(\frac{\partial \xi}{\partial x}\right)^2 \left(\frac{\partial^2}{\partial \xi^2}\right) \quad (20)$$

then,

$$\frac{\partial^2 T}{\partial x^2} = \frac{\partial^2 \xi}{\partial x^2} \frac{\partial T}{\partial \xi} + \left(\frac{\partial \xi}{\partial x}\right)^2 \frac{\partial^2 T}{\partial \xi^2} \quad (21)$$

For $\xi = \cos^{-1}(1 - x/L_x)$, we have

$$\frac{\partial \xi}{\partial x} = \frac{1}{\sqrt{2xL_x - x^2}} \quad (22)$$

$$\frac{\partial^2 \xi}{\partial x^2} = \frac{-(L_x - x)}{\sqrt{(2xL_x - x^2)^3}} \quad (23)$$

the heat equation in (ξ, t) coordinate system is

$$\frac{\partial T}{\partial t} = \alpha \left[\frac{\partial^2 \xi}{\partial x^2} \frac{\partial T}{\partial \xi} + \left(\frac{\partial \xi}{\partial x}\right)^2 \frac{\partial^2 T}{\partial \xi^2} \right] + S[L_x(1 - \cos \xi)] \quad (24)$$

discretization form is

$$\begin{aligned} \frac{T_j^{n+1} - T_j^n}{\Delta t} &= \alpha \left[\frac{-(L_x - X_j)}{\sqrt{(2X_j L_x - X_j^2)^3}} \frac{T_{j+1}^n - T_{j-1}^n}{2\Delta \xi} + \frac{1}{(2X_j L_x - X_j^2)} \frac{T_{j+1}^{n+1} - 2T_j^n + T_j^{n-1}}{(\Delta \xi)^2} \right] \\ &\quad + S[L_x(1 - \cos \xi_j)] \end{aligned} \quad (25)$$

The numerical results is shown in Fig.8. It should be pointed out that Fig.8 looks much like Fig.7. The difference is that here the calculation of T is based on a uniform grid ξ , while in Problem 2(3) calculation is on a non-uniform grid x .

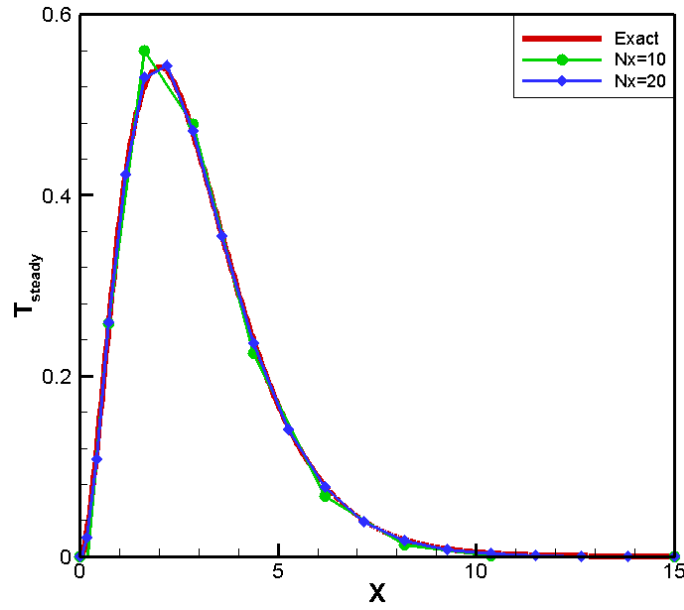


Figure 8: Results of FTCS with different uniform mesh grids (after coordinate transformation)

2.5 Crank-Nicolson Method

Using Crank-Nicolson method for time advancement,

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{\frac{1}{2}(T_{i+1}^{n+1} + T_{i+1}^n) - 2 \cdot \frac{1}{2}(T_i^{n+1} + T_i^n) + \frac{1}{2}(T_{i-1}^{n+1} + T_{i-1}^n)}{(\Delta x)^2} + S(X_i) \quad (26)$$

then, we have

$$\frac{\alpha \Delta t}{2(\Delta x)^2} T_{i-1}^{n+1} - [1 + \frac{\alpha \Delta t}{(\Delta x)^2}] T_i^{n+1} + \frac{\alpha \Delta t}{2(\Delta x)^2} T_{i+1}^{n+1} = -T_i^n - \frac{\alpha \Delta t}{2(\Delta x)^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n) - S(X_i) \Delta t \quad (27)$$

Define

$$\begin{aligned} A &= \frac{\alpha \Delta t}{2(\Delta x)^2} \\ B &= -[1 + \frac{\alpha \Delta t}{(\Delta x)^2}] \\ C &= \frac{\alpha \Delta t}{2(\Delta x)^2} \\ K_i &= -T_i^n - \frac{\alpha \Delta t}{2(\Delta x)^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n) - S(X_i) \Delta t \end{aligned} \quad (28)$$

then, Eq.27 is denoted as

$$AT_{i-1}^{n+1} + BT_i^{n+1} + CT_{i+1}^{n+1} = K_i \quad (29)$$

The Thomas algorithm will be employed to solve above tridiagonal systems of equations.

The numerical results is shown in Fig.9.

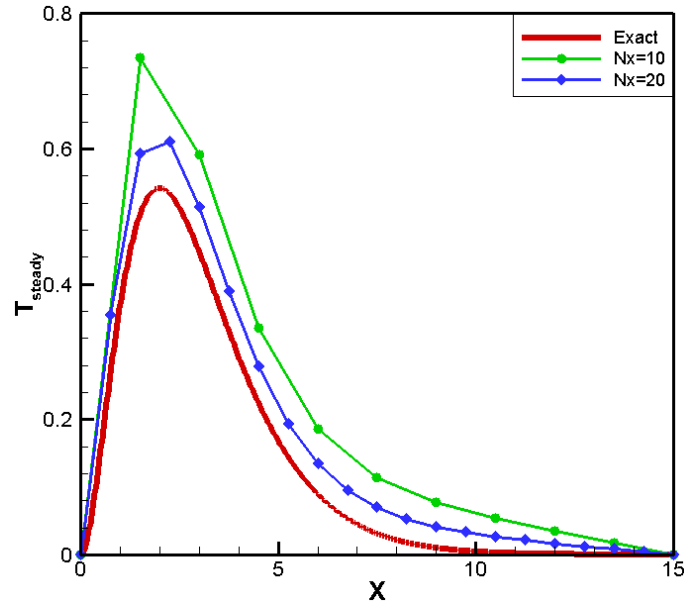


Figure 9: Results of Crank-Nicolson method on uniform mesh grids

2.6 Discussion

For each method mentioned above, given grid points $N_x = 20$.

The convergence criterion is

$$\frac{|T(t) - T(t-2)|}{\sum |T(t)|} \leq 10^{-7} \quad (30)$$

1. Find the maximum time step required for stable solutions.

Table 1: Comparison of different methods

	FTCS	Non-uniform grid	coordinate transform	Crank-Nicolson
$(\Delta t)_{\max}$	0.51	0.006	0.009	≥ 1.0
iteration	80	29460	20656	290

2. Plot transient solutions at $t = 2$ and $t = 10$ as shown in Fig.10.

- We compare different methods at $t = 2$, at least 2 time steps are required, thus, we set $\Delta t = 1.0$ for Crank-Nicolson. Actually, Δt can be much larger

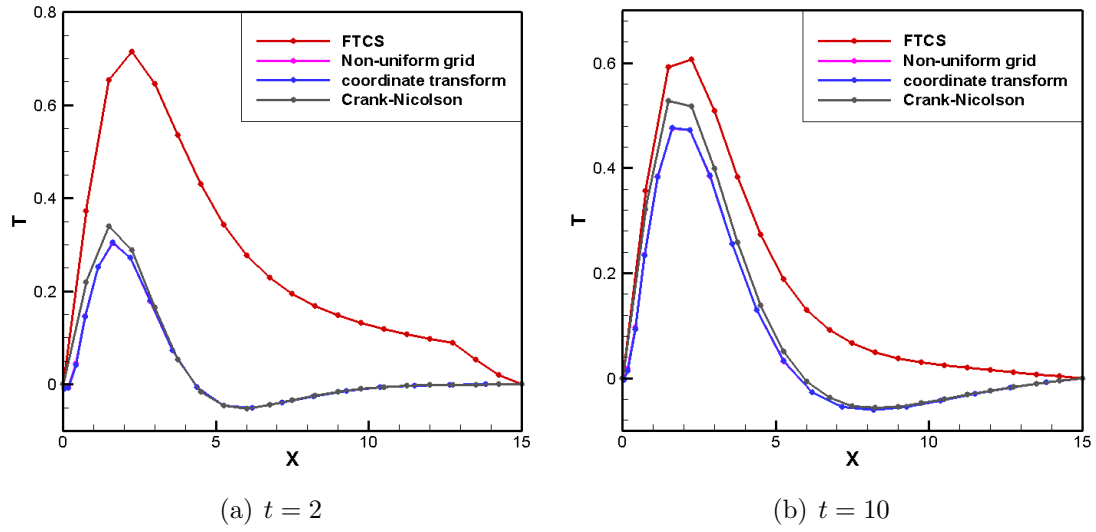


Figure 10: Comparison accuracy of different methods at $t = 2$ and $t = 10$

than 1.0 for Crank-Nicolson scheme since Crank-Nicolson scheme is unconditionally stable.

- FTCS scheme shows the largest discrepancy among all the test methods under unsteady condition, because the error is $O((\Delta x)^2, \Delta t)$.
- Using non-uniform grid, i.e., put more mesh points in the region where solutions change rapidly, will help reduce the error.

3 2D Steady-state Heat Equation

Solve steady-state 2D heat conduction equation in unit square.

Boundary condition:

- at $x = 0$, $T = 0$.
- at $x = 1$, $T = 0$.
- at $y = 0$, $\frac{\partial T}{\partial y} = 0$.
- at $y = 1$, $T = \sin(\pi x)$.

The analytical solution can be obtained by variable separation

$$T_{exact} = \frac{\cosh(\pi y)}{\cosh(\pi)} \sin(\pi x) \quad (31)$$

2D heat equation is

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \quad (32)$$

steady state can be obtained when $t \rightarrow \infty$ thus $\partial T / \partial t = 0$.

The convergence criterion for the solution to reach steady state is

$$\frac{|T(t) - T(t - 100)|}{\sum |T(t)|} \leq 10^{-7} \quad (33)$$

Discretization of heat equation:

$$\frac{T_{i,j}^{n+1} - T_{i,j}^n}{\Delta t} = \alpha \left[\frac{T_{i+1,j}^n - 2T_{i,j}^n + T_{i-1,j}^n}{(\Delta x)^2} + \frac{T_{i,j+1}^n - 2T_{i,j}^n + T_{i,j-1}^n}{(\Delta y)^2} \right] \quad (34)$$

Discretization of Neumann boundary condition:

$$\left(\frac{\partial T}{\partial y} \right)_{j=1} = \frac{-3T_{i,1} + 4T_{i,2} - T_{i,3}}{\Delta y} = 0 \quad (35)$$

thus,

$$T_{i,1} = \frac{4T_{i,2} - T_{i,3}}{3} \quad (36)$$

Here is the main code snippets:

```

1
2     do j=2,ny-1
3         do i=2,nx-1
4             T(i,j) = T(i,j)+dt*alpha*( (T(i+1,j)-2.0d0*T(i,j)+T(i-1,j))/dx/dx+(T(i,j+1)-2.0d0*T(i,j)+T(i,j-1))/dy/dy )

```

```

5         enddo
6     enddo
7
8     ! Left and right side B.C.
9     do j=1,ny
10        T(1,j) = 0.0d0
11        T(nx,j) = 0.0d0
12    enddo
13    ! Top and bottom side B.C.
14    do i=1,nx
15        T(i,1) = (4.0d0*T(i,2)-T(i,3))/3.0d0
16        T(i,ny) = dsin(Pi*X(i))
17    enddo

```

The temperature field shown in Fig.11.

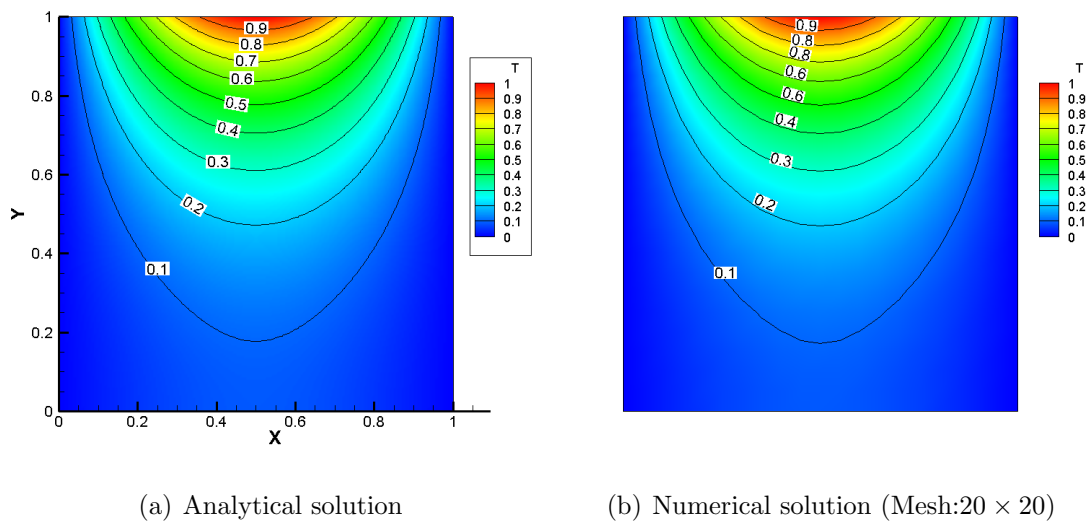


Figure 11: Steady-state 2D heat conduction

Comparison of center temperature with the exact solution shown in Fig.12

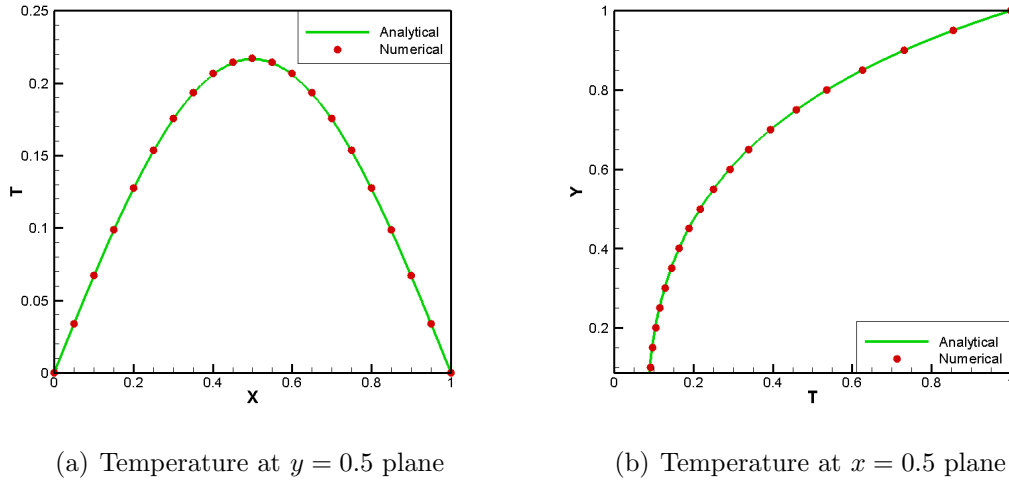


Figure 12: Comparison of center temperature with analytical solution

4 MacCormack Method for Burgers Equation

Solve linearized Burgers equation $u_t + cu_x = \mu u_{xx}$, $c = 0.5$, $\mu = 0.02$.

Initial condition $u(x, 0) = 0$, $0 \leq x \leq 1$.

Boundary condition $u(0, t) = 100$, $u(1, t) = 0$.

Choose $\Delta x = 0.02$ and $\Delta t = 0.001$.

The exact solution for steady-state is

$$u(x) = 100 \frac{1 - \exp[25(x - 1)]}{1 - \exp(-25)} \quad (37)$$

Use MacCormack method, discretization is

$$\begin{aligned} \text{Predictor : } \overline{u_j^{n+1}} &= u_j^n - c \frac{\Delta t}{\Delta x} (u_{j+1}^n - u_j^n) + \frac{\mu \Delta t}{(\Delta x)^2} (u_{j+1}^n - 2u_j^n + u_{j-1}^n) \\ \text{Corrector : } u_j^{n+1} &= \frac{1}{2} [u_j^n + \overline{u_j^{n+1}} - c \frac{\Delta t}{\Delta x} (\overline{u_j^{n+1}} - \overline{u_{j-1}^{n+1}}) + \frac{\mu \Delta t}{(\Delta x)^2} (\overline{u_{j+1}^{n+1}} - 2\overline{u_j^{n+1}} + \overline{u_{j-1}^{n+1}})] \end{aligned} \quad (38)$$

Here is the main code snippets:

```

1
2     ! predictor
3     do i=1,nx-1
4         uPre(i) = u(i)-constC*dt/dx*(u(i+1)-u(i))+nu*dt/dx/dx*(u(
5             i+1)-2.0d0*u(i)+u(i-1))
6     enddo
7     uPre(0) = 100.0d0
8     uPre(nx) = 0.0d0

```

```

8
9      ! corrector
10     do i=1,nx-1
11         u(i) = 0.5d0*( u(i)+uPre(i)-constC*dt/dx*(uPre(i)-uPre(i
            -1))+nu*dt/dx/dx*(uPre(i+1)-2.0d0*uPre(i)+uPre(i-1)) )
12     enddo
13
14     u(0) = 100.0d0
15     u(nx) = 0.0d0

```

The results shown in Fig.13.

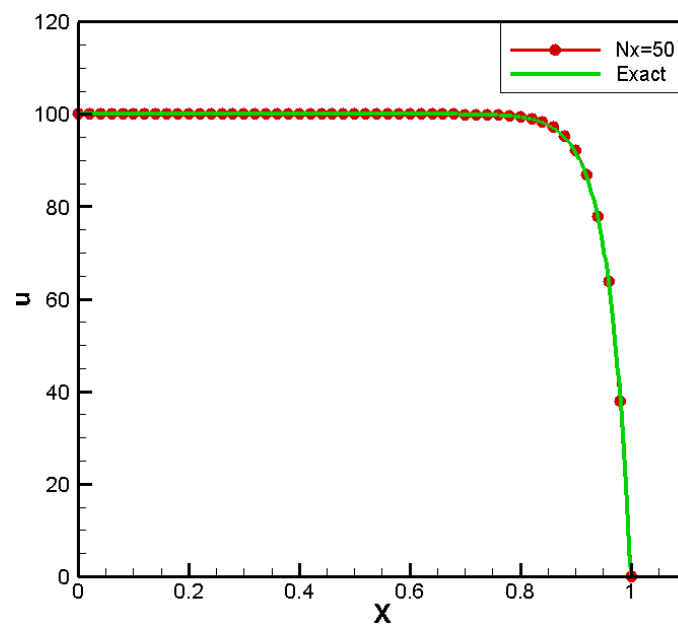


Figure 13: MacCormack method for linearized Burgers equation ($N_x = 50$)