Dicretization of Partial Differential Equations (CLW: 7.2, 7.3)

We will follow a procedure similar to the one used in the previous class.
We consider the unsteady vorticity transport equation, noting that the equation is non-linear.
Vorticity vector: \( \vec{\xi} = \text{curl} \vec{\nu} = \vec{\nabla} \times \vec{\nu} \)

\[
= \begin{vmatrix}
\hat{i} & \hat{j} & \hat{k} \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
u & v & w
\end{vmatrix}
\]

Is a measure of rotational effects.
\( \vec{\xi} = 2\vec{\omega} \) where \( \vec{\omega} \) is the local angular velocity of a fluid element.

For 2-D incompressible flow, the vorticity transport equation is given by

\[
\frac{\partial \vec{\xi}}{\partial t} + u \frac{\partial \vec{\xi}}{\partial x} + v \frac{\partial \vec{\xi}}{\partial y} = \nu \nabla^2 \vec{\xi}
\]  

\[
\nabla^2 \vec{\xi} = \frac{\partial^2 \vec{\xi}}{\partial x^2} + \frac{\partial^2 \vec{\xi}}{\partial y^2}
\]

\( \nu \) - kinematic viscosity \( \left( \equiv \frac{\mu}{\rho} \right) \frac{\text{m}^2}{\text{s}} \)
As in the case of ODE, the partial derivatives can be discretized using Taylor series

\[ u(x + h, y + k) = u(x, y) + \left(h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y}\right) u(x, y) + \]

\[ \frac{1}{2!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y}\right)^2 u(x, y) + \ldots \]

\[ \frac{1}{(n-1)!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y}\right)^{n-1} u(x, y) + R_n \]  

\[ R_n = O\left[ \left( |h| + |k| \right)^n \right] \]

We can expand in Taylor series for the 8 neighboring points of \((i,j)\) using \((i,j)\) as the central point.
\[ u_{i-1,j} = u_{i,j} - \Delta x u_x + \frac{(\Delta x)^2}{2!} u_{xx} - \frac{(\Delta x)^3}{3!} u_{xxx} \]  \hspace{1cm} (4) \\
\[ u_{i+1,j} = u_{i,j} + \Delta x u_x + \frac{(\Delta x)^2}{2!} u_{xx} + \frac{(\Delta x)^3}{3!} u_{xxx} \]  \hspace{1cm} (5)

Here \( u_x = \frac{\partial u}{\partial x} \), \( u_{xx} = \frac{\partial^2 u}{\partial x^2} \) etc.

Note: all derivatives are evaluated at \((i,j)\)

Rearranging the equations yield the following finite difference formulas for the derivatives at \((i,j)\).

\[ \frac{\partial u}{\partial x} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + \mathcal{O} (\Delta x) \]  \hspace{1cm} (6)
Eq.(6) is known as the forward difference formula.

Eq.(7) is known as the backward difference formula.

Eq.(8) and (9) are known as central difference formulas.

Compact notation:

\[ \delta_x u_{i,j} = \frac{u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}}{\Delta x} \]  

(10)
The Heat conduction problem (ID)

Consider unit area in the direction normal to x. Energy balance for a CV of cross section of area 1 and length Δx:

Volume of CV, \( \text{d}V = 1 \Delta x \)

Change in temperature during time interval \( \Delta t \), \( \Delta T \)

Increase in energy of CV:

\[
\rho \Delta x \left[ c_p \frac{\partial T}{\partial t} \right] \Delta t + \text{HOT}
\]

This should be equal to the net heat transfer across the two faces:

\[
- k \frac{\partial T}{\partial x} \bigg|_x \Delta t - \left[ - k \frac{\partial T}{\partial x} \bigg|_x + \frac{\partial}{\partial x} \left( - k \frac{\partial T}{\partial x} \right) \bigg|_x \right] \Delta x \Delta t + \text{HOT}
\]
Equating the two and canceling $\Delta t \Delta x$ gives

$$\rho c_p \frac{\partial T}{\partial t} = -\frac{\partial}{\partial x} \left( -k \frac{\partial T}{\partial x} \right)$$

Note: higher order terms (HOT) have been dropped.
If we assume $k=\text{constant}$, we get

$$\rho c_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}$$

Or

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_p} \frac{\partial^2 T}{\partial x^2} = \alpha \frac{\partial^2 T}{\partial x^2}$$

Where $\alpha \equiv \frac{k}{\rho c_p}$ is the thermal diffusivity.

Letting $\xi = x/L$, and $\tau = \alpha t/L^2$, the above equation becomes

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2}$$
The above is a Parabolic Partial Differential Equation.

\[ \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \]  

(11)

Physical problem

A rod insulated on the sides with a given temperature distribution at time \( t = 0 \).
Rod ends are maintained at specified temperature at all time.
Solution \( u(x,t) \) will provide temperature distribution along the rod
At any time \( t > 0 \).

\[ \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad 0 < x < l, \quad 0 < t < t_1 \]
IC:
\[ u(x, 0) = f(x) \quad 0 \leq x \leq l \]  
(12)

BC:
\[ u(0, t) = g_0(t) \quad 0 < t \leq t_1 \]
\[ u(l, t) = g_1(t) \quad 0 < t \leq t_1 \]  
(13)

Difference Equation

Solution involves establishing a network of Grid points as shown in the figure in the next slide.

Grid spacing:
\[ \Delta x = \frac{l}{M}, \quad \Delta t = \frac{t_1}{N} \]
M, N are integer values chosen based on required accuracy and available computational resources.

Explicit form of the difference equation

\[
\frac{u_{i,n+1} - u_{i,n}}{\Delta t} = \frac{u_{i-1,n} - 2u_{i,n} + u_{i+1,n}}{(\Delta x)^2}
\]  \hspace{1cm} (14)

Define \[ \lambda = \frac{\Delta t}{(\Delta x)^2} \]
Then

\[ u_{i,n+1} = \lambda u_{i-1,n} + (1 - 2\lambda) u_{i,n} + \lambda u_{i+1,n} \quad (15) \]

Circles indicate grid points involved in space difference
Crosses indicate grid points involved in time difference.

Note:
At time \( t=0 \) all values \( u_{i,0} = f(x_i) \) are known (IC).

In eq.(15) if all \( u_{i,n} \) are known at time level \( n \), \( u_{i,n+1} \) can be calculated explicitly.

Thus all the values at a time level \((n+1)\) must be calculated before advancing to the next time level.

Note: If all IC and BC do not match at \((0,0)\) and \((l,0)\), it should be handled in the numerical procedure.
Select one or the other for the numerical calculation.
There will be a small error present because of this inconsistency.
Convergence of Explicit Form.

Remember that the finite difference form is an approximation. The solution also will be an approximation.

The error introduced due to only a finite number of terms in the Taylor series is known as truncation error, \( \varepsilon \).

The solution is said to converge if

\[
\varepsilon \rightarrow 0 \quad \text{when} \quad \Delta x, \Delta t \rightarrow 0
\]

Error is also introduced because variables are represented by a finite number of digits in the computer. This is known as round-off error.

For the explicit method, the truncation error, \( \varepsilon \) is

\[
\varepsilon = O[\Delta t]
\]

The convergence criterion for the explicit method is as follows:

\[
0 < \lambda \leq \frac{1}{2} \quad \text{where} \quad \lambda = \frac{\Delta t}{(\Delta x)^2}
\]