



ME/AE 339

# Computational Fluid Dynamics

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## Topic3\_PDE

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Topic 3 Discretization of PDE

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Computational Fluid Dynamics (AE/ME 339)

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### Discretization 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.

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Vorticity vector:  $\bar{\xi} = \text{curl } \bar{v} = \bar{\nabla} \times \bar{v}$

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

Is a measure of rotational effects.

$\bar{\xi} = 2\bar{\omega}$  where  $\bar{\omega}$  is the local angular velocity of a fluid element.

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

$$\frac{\partial \bar{\xi}}{\partial t} + u \frac{\partial \bar{\xi}}{\partial x} + v \frac{\partial \bar{\xi}}{\partial y} = \nu \nabla^2 \bar{\xi} \quad (1)$$

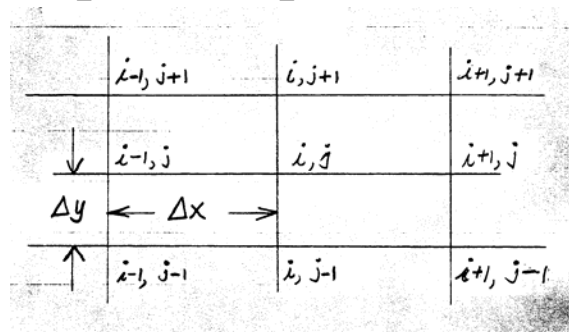
$$\nabla^2 \bar{\xi} \equiv \frac{\partial^2 \bar{\xi}}{\partial x^2} + \frac{\partial^2 \bar{\xi}}{\partial y^2}$$

$$\nu - \text{kinematic viscosity} \quad \left( \equiv \frac{\mu}{\rho} \right) \frac{m^2}{s}$$

As in the case of ODE ,the partial derivatives can be discretized  
Using Taylor series

$$\begin{aligned}
 u(x+h, y+k) &= u(x, y) + \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right) u(x, y) + \\
 &\frac{1}{2!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^2 u(x, y) + \dots \\
 &\frac{1}{(n-1)!} \left( h \frac{\partial}{\partial x} + k \frac{\partial}{\partial y} \right)^{n-1} u(x, y) + R_n
 \end{aligned} \tag{2}$$

$$R_n = O \left[ (|h| + |k|)^n \right] \tag{3}$$



We can expand in Taylor series for the 8 neighboring points of  
(i,j) using (i,j) as the central point.

$$u_{i-1,j} = u_{i,j} - \Delta x u_x + \frac{(\Delta x)^2}{2!} u_{xx} - \frac{(\Delta x)^3}{3!} u_{xxx} \quad (4)$$

$$u_{i+1,j} = u_{i,j} + \Delta x u_x + \frac{(\Delta x)^2}{2!} u_{xx} + \frac{(\Delta x)^3}{3!} u_{xxx} \quad (5)$$

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).

$$\frac{\partial u}{\partial x} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x) \quad (6)$$

$$\frac{\partial u}{\partial x} = \frac{u_{i,j} - u_{i-1,j}}{\Delta x} + O(\Delta x) \quad (7)$$

$$\frac{\partial u}{\partial x} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O[(\Delta x)^2] \quad (8)$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\Delta x)^2} + O[(\Delta x)^2] \quad (9)$$

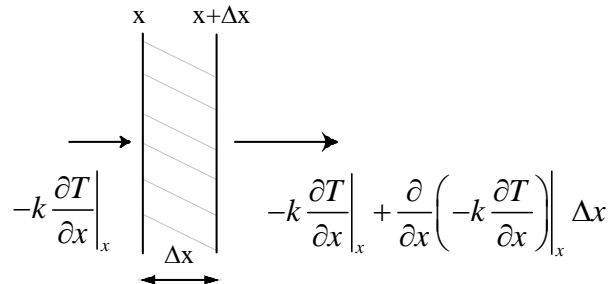
Eq.(6) is known as the forward difference formula.

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

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

Compact notation:

$$\delta_x u_{i,j} = \frac{u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}}{\Delta x} \quad (10)$$

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  $\Delta x$ :

Volume of CV,  $dV = 1 \Delta x$

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Change in temperature during time interval  $\Delta t$ ,  $\Delta T = \Delta T$

Increase in energy of CV :

$$\rho \Delta x 1 c_p \frac{\partial T}{\partial t} \Delta t + HOT$$

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

$$-k \frac{\partial T}{\partial x} \Big|_x \Delta t - \left[ -k \frac{\partial T}{\partial x} \Big|_{x+\Delta x} + \frac{\partial}{\partial x} \left( -k \frac{\partial T}{\partial x} \right) \Big|_x \Delta x \right] \Delta t + HOT$$

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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

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

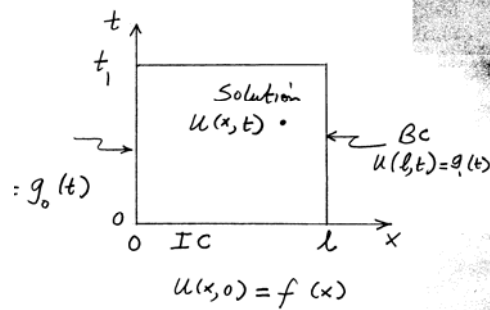
Or 
$$\frac{\partial T}{\partial t} = \frac{k}{\rho c_p} \frac{\partial^2 T}{\partial x^2} = \alpha \frac{\partial^2 T}{\partial x^2}$$

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.



$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad (11)$$

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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  $t > 0$ .

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad 0 < x < l, 0 < t < t_1$$

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IC:

$$u(x, 0) = f(x) \quad \boxed{0 \leq x \leq l} \quad (12)$$

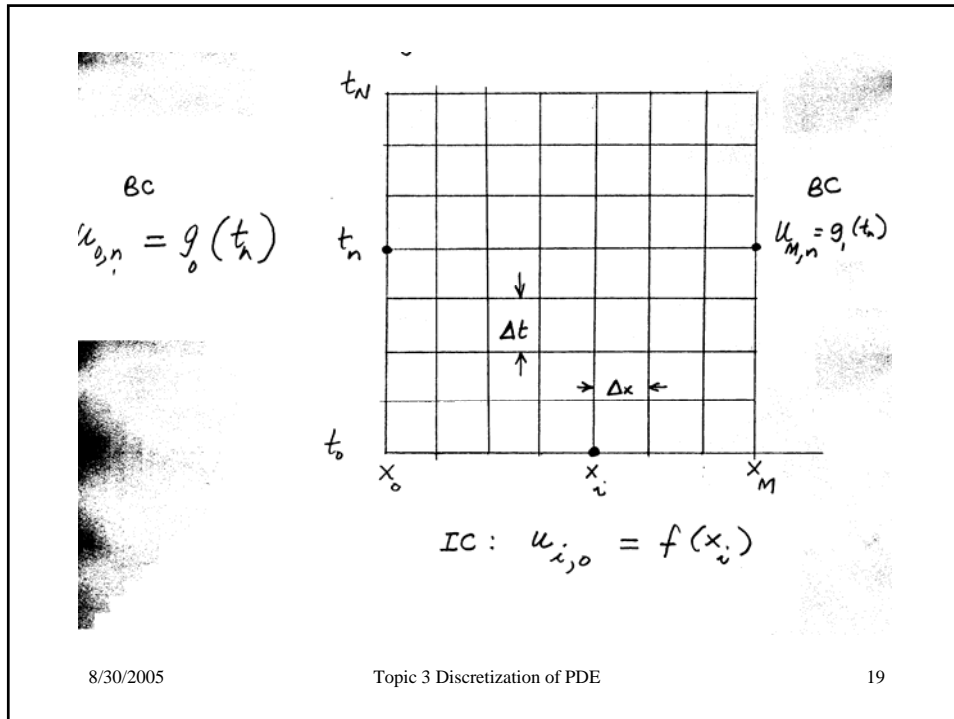
BC:

$$\begin{aligned} u(0, t) &= g_0(t) & 0 < t \leq t_1 \\ u(l, t) &= g_1(t) & 0 < t \leq t_1 \end{aligned} \quad (13)$$

### Difference Equation

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

$$\text{Grid spacing:} \quad \Delta x = \frac{l}{M}, \quad \Delta t = \frac{t_1}{N}$$



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M,N are integer values chosen based on required accuracy and available computational resources.

Explicit form of the difference equation

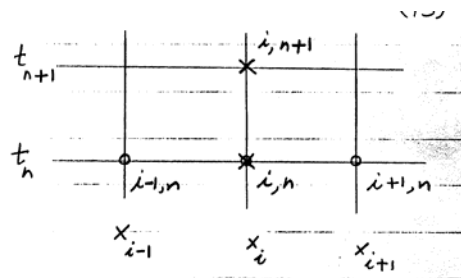
$$\frac{u_{i,n+1} - u_{i,n}}{\Delta t} = \frac{u_{i-1,n} - 2u_{i,n} + u_{i+1,n}}{(\Delta x)^2} \quad (14)$$

Define  $\lambda = \frac{\Delta t}{(\Delta x)^2}$

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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:

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



# ***Program Completed***

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