AE/ME 339

Computational Fluid Dynamics (CFD)

K. M. Isaac
Professor of Aerospace Engineering
Partial Differential Equations (PDE) (CLW: 7.1, 7.3, 7.4)

PDE’s can be linear or nonlinear
Order: Determined by the order of the highest derivative.
Linear, 2\text{nd} order PDE’s are classified as the elliptic, hyperbolic
Parabolic type.

Example:

\[
A_1 \frac{\partial^2 u}{\partial x^2} + A_2 \frac{\partial^2 u}{\partial y^2} + A_3 \frac{\partial^2 u}{\partial z^2} + B_1 \frac{\partial u}{\partial x} \\
+ B_2 \frac{\partial u}{\partial y} + B_3 \frac{\partial u}{\partial z} + Cu + D = 0
\]
Coefficients \( A_1, A_2, A_3 \) May be +1, -1 or zero.

\( u \) is the dependent variable and \( x, y, z \) are the independent variables. Note that we do not have any cross-derivative terms.

Classification:

Elliptic: \( A_1, A_2, A_3 \) are non-zero and have the same sign, then PDE is of the elliptic type.
Hyperbolic:

\[ A_1, A_2, A_3 \] are non-zero and of mixed sign, the PDE is hyperbolic

Parabolic:

If one of \[ A_1, A_2, A_3 \] say \[ A_2 \] is zero and the rest are of the same sign, and if \[ B_2 \] is non-zero, the PDE is parabolic.

Since \( A_i, B_i, C \) and \( D \) may be functions of \( x, y \) and \( z \), the classification may depend on position in space.

In many CFD problems, one of the independent variables will be time and the rest will be space coordinates such as \( x, y, z \) or or transformed variables such as \( \xi, \eta, \zeta \).
Examples

Elliptic
\[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \]

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

Parabolic
\[ \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \]
Numerical solution of PDE requires a finite number of points to discretize the equations.
Examples:

See Figure in the next slide.
Solution requires initial and boundary conditions depending on the Problem.
Indices i, j, n can be used to label the nodes in x, y, t directions (see fig.)
If the origin has i=0, j=0 and n = 0, then the node i, j, n has coordinates $i\Delta x, j\Delta y, n\Delta t,$

where $\Delta x, \Delta y, \Delta t$ are the uniform intervals between nodes along x, y, t coordinate directions.
Let $u(x, y, t) \equiv u_{i,j,n}$ be the exact solution of the PDE and $V_{i,j,n}$ be the approximations to be determined at each grid point.
The derivatives of the original PDE are approximated using the symbol 
\[ V_{i, j, n} \] and the discretization intervals \( \Delta x, \Delta y, \Delta t \).

The procedure leads to a set of algebraic equations of which are then solved.

Fine grids can be used to obtain solutions \( V_{i, j, n} \) that are close to \( U_{i, j, n} \).

Examples of PDE’s common in engineering

1. Unsteady heat conduction equation

1D form:
\[
\frac{\partial}{\partial x} \left( k \frac{\partial T}{\partial x} \right) = c_p \rho \frac{\partial T}{\partial t}
\]
T - temperature
\(k\) - thermal conductivity
\(\rho\) - density
\(c_p\) - specific heat

If \(k\) is a constant, the equation becomes

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

Where \(\alpha \equiv \frac{k}{c_p \rho}\) is the thermal diffusivity.
In CFD, normalization of variables are often used to improve the solution (for proper scaling of the variables).

Let \( \xi = \frac{x}{L}, \tau = \frac{\alpha t}{L^2} \)

for heat conduction in a rod of length L.

The PDE then becomes

\[
\frac{\partial^2 T}{\partial \xi^2} = \frac{\partial T}{\partial \tau}
\]

It is also possible to non-dimensionalize the dependent variable T.
Taylor’s Expansion.

Let \( \frac{dy}{dx} = f(x, y) \). Taylor series is as follows. \( y(x_0 + h) = y(x_0) + hf \left( x_0, y \left( x_0 \right) \right) + \frac{h^2}{2!} f' \left( x_0, y \left( x_0 \right) \right) \)

\[ + \frac{h^3}{3!} f'' \left( x_0, y \left( x_0 \right) \right) + \ldots \] \( (2) \)

Where \( f' \left( x, y \left( x \right) \right) = \frac{df}{dx} \left( x, y \left( x \right) \right) \)

\[ f'' \left( x, y \left( x \right) \right) = \frac{d^2 f}{dx^2} \left( x, y \left( x \right) \right) \]
The higher order derivatives in Eq.(2) can be determined by Differentiating Eq.(1) by chain rule. i.e.,

\[
\frac{df}{dx} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} \cdot \frac{dy}{dx}
\]

Example 1: \(f(x,y)\) is a function of \(x\) alone.

\[
\frac{dy}{dx} = x^2
\]
\[ f'(x, y) = 2x \]
\[ f''(x, y) = 2 \]
\[ f'''(x, y) = 0 \]
\[ f^n(x, y) = 0 \]
\[ f'(x_0, y_0) = 2x_0 \]
\[ f''(x_0, y_0) = 2 \]
\[ f'''(x_0, y_0) = 0 \]
\[ f^n(x_0, y_0) = 0 \]
The function at the neighboring point \((x = x_0 + h)\) becomes

\[
y(x_0 + h) = y(x_0) + hx_0^2 + hx_0 + \frac{h^3}{3}
\]

Example 2: \(f(x,y)\) is a function of \(y\) alone.

\[
\frac{dy}{dx} = f(x, y) = 2y
\]
\[ f'(x, y) = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} \frac{dy}{dx} = 2y + 2y = 4y \]

Similarly

\[ f''(x, y) = 8y \]
\[ f'''(x, y) = 16y \]
\[ f^n(x, y) = 2^{(n+1)}y \]
\[ y(x_0 + h) = y(x_0) + 2h y(x_0) + 4 \frac{h^2}{2!} y(x_0) + 8 \frac{h^3}{3!} y(x_0) \]

\[ = y(x_0) \left[ 1 + 2h + \frac{(2h)^2}{2!} + \frac{(2h)^3}{3!} + \ldots \right] \]
Taylor series can also be used for non-linear higher order equations.

Example:

\[
\frac{d^2 y}{dx^2} - \frac{dy}{dx} + xy^2 = 0
\]

\[
\frac{dy}{dx} = f(x, y) = \frac{d^2 y}{dx^2} + xy^2
\]

\[
y''' = y'' - xy^2
\]

\[
y'''' = y''' - 2xyy' - y^2
\]
Consider the initial conditions

\[ y^{'''} = y^{'''} - (2yy' + 2xyy'' + 2xy'^2) - 2yy' \]
\[ y^{'''} = y^{'''} - 4yy' - 2xy'^2 - 2xyy'' \]

At \( x = 0, \ y(0) = 1, \ y'(0) = -1 \)
\[
y''(0) = y'(0) - 0 \times y^2(0) = -1
\]
\[
y'''(0) = y''(0) - y^2(0)
\]
\[
y'''(0) = -1 - 1 = -2
\]
\[
y^{iv}(0) = y'''(0) - 4 \times 1(-1)
\]
\[
y^{iv}(0) = -2 + 4 = 2
\]
Since Taylor series gives

\[ y_{k+1} = y_k + y_k' \frac{h}{1!} + y_k'' \frac{h^2}{2!} + y_k''' \frac{h^3}{3!} + \cdots \]

For \( k = 0 \), \( y_1 \) becomes

\[ y_1 = 1 - h - \frac{h^2}{2!} - \frac{h^3}{3!} + \frac{h^4}{4!} + \cdots \]

Letting \( h = 0.1 \), we get

\[ y_1 = 1 - 0.1 - \frac{0.01}{2} - \frac{0.001}{3} + \frac{0.0001}{12} \]

\[ y_1 = 0.894675 \]
Calculation of $y_2$

Need $y_1'$

Calculate $y_1'$ by differentiating the expression for $y_1$ w.r.t. $h$.

$$y_1' = -1 - h - h^2 + \frac{h^3}{3} + \ldots$$

$$y_1' = -1 - 0.1 - 0.01 + \frac{0.001}{3} = -1.1097$$

$y_1''$, $y_1'''$, $y_1^{iv}$ etc. can now be calculated as before and $y_2$ can be obtained.