AE/ME 339

Computational Fluid Dynamics (CFD)

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Crank-Nicolson Method

Crank-Nicolson method

Previous explicit and implicit methods have discretization error

$$\varepsilon = O\left[\Delta t, (\Delta x)^2\right]$$

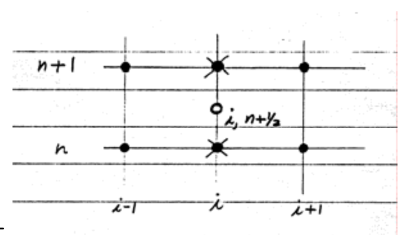
Recall, the central difference formula:

$$\frac{\partial u}{\partial t} = \frac{u_{i,n+1} - u_{i,n-1}}{2\Delta t} + O[(\Delta t)^2]$$

Define the central difference operators

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

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



Let us now try the following form for the second derivative

$$\frac{\partial^2 u}{\partial x^2} = \delta_x^{\,2} u_{i,n+1}\theta + (1-\theta)\delta_x^{\,2} u_{i,n}$$

The above form involves 6 points to represent $\frac{\partial^2 u}{\partial x^2}$

And θ lies in the range: $0 \le \theta \le 1$

Depending on the value of θ, the method will be explicit (θ = 0), implicit (θ = 1), or a combination of the two.

For the Crank–Nicolson (C-N) method, θ = ½.
The difference equation now becomes

$$\frac{u_{i,n+1} - u_{i,n}}{\Delta t} = \frac{1}{2}\delta_x^{\ 2} u_{i,n+1} + \frac{1}{2}\delta_x^{\ 2} u_{i,n}$$

C-N method has the following properties:
i) Stable for <u>all values</u> of the ratio, $\lambda = \Delta t/(\Delta x)^2$

(ii) Has truncation error $O\left[(\Delta t)^2, (\Delta x)^2\right]$

When written in full, the equation becomes

$$-\lambda u_{i-1,n+1} + 2(1+\lambda)u_{i,n+1} - \lambda u_{i+1,n+1} =$$

$$\lambda u_{i-1,n} + 2(1-\lambda)u_{i,n} + \lambda u_{i+1,n}$$

Dufort-Frankel Method (7.13)

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

Method is an unconditionally stable, explicit method

3 time levels are involved
More difficult to formulate IC
More computer storage is required

Error $O\left[(\Delta t)^2, (\Delta x)^2\right]$

Alternating-Direction Implicit (ADI) Method (7.14)

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Alternating-Direction Implicit (ADI) Method (7.14)

The unsteady state heat conduction in a slab is governed by the following equation

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

Figure

Top and bottom surfaces are Insulated

BC are imposed on the 4 sides

Explicit Method

$$\frac{u_{i,j,n+1} - u_{i,j,n}}{\Delta t} = \delta_x^2 u_{i,j,n} + \delta_y^2 u_{i,j,n}$$

Stability Criterion: $\Delta t \le \frac{1}{2\left[(\Delta x)^{-2} + (\Delta y)^{-2}\right]}$

Implicit Method

$$\frac{u_{i,j,n+1} - u_{i,j,n}}{\Delta t} = \delta_x^2 u_{i,j,n+1} + \delta_y^2 u_{i,j,n+1}$$

Writing in full with $\Delta x = \Delta y$ yields

$$-\lambda u_{i-1,j,n+1} - \lambda u_{i,j-1,n+1} + (1+4\lambda) u_{i,j,n+1} - \lambda u_{i,j+1,n+1}$$
$$-\lambda u_{i+1,j,n+1} = u_{i,j,n}$$

Scheme is stable for all values of λ

There are 5 unknowns per equation
Gauss elimination for solution is more complicated
System is not tri-diagonal

ADI Method

Let us now consider a parabolic PDE in two dimensions denoted by x and y i.e.,

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

ADI uses two finite difference equations used in turn over successive time steps each of size Δt/2

The first equation is implicit only in the x-direction
Second equation is implicit only in the y-direction

$u_{i,j}^{*}$ is an intermediate value at the end of time step Δt/2

Step 1
$$\frac{u_{i,j}^{*} - u_{i,j,n}}{(\Delta t / 2)} = \delta_x^2 u_{i,j}^{*} + \delta_y^2 u_{i,j,n}$$

Another way of writing: $u_{i,j}^{*} \equiv u_{i,j}^{n+1/2}$

Step 2
$$\frac{u_{i,j,n+1} - u_{i,j}^{*}}{(\Delta t/2)} = \delta_x^2 u_{i,j}^{*} + \delta_y^2 u_{i,j,n+1}$$

$u_{i,j}^{*}$ values are solved for in the first step and

$u_{i,j,n+1}$ values are solved for in the second step

Advantage is that the matrices in both steps are still tri-diagonal

Exercise: Write the equations in full using

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

Can be shown that procedure is unconditionally stable

Discretization error $O\left[(\Delta t)^2, (\Delta x)^2\right]$

ADI can also be used for solving elliptic PDE's

ADI is not recommended for 3D problems

Example

An infinitely long bar has thermal diffusity

$$\alpha = \frac{k}{\rho c_p}$$

Square cross section of side 2a
IC: Temperature is uniform at T_0
BC: side surface temperature T_1

Figure

Compute temperature distribution T(x,y,t) inside the slab

Can write $$\rho c_p \frac{\partial T}{\partial t} = k\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right]$$

Procedure

Non-dimensionalize the equations as follows

$$X = \frac{x}{a}, \qquad Y = \frac{y}{a}, \qquad \tau = \frac{\alpha t}{a^2}, \qquad \theta = \frac{T - T_0}{T_1 - T_0}$$

$$\frac{\partial \theta}{\partial \tau} = \frac{\partial^2 \theta}{\partial X^2} + \frac{\partial^2 \theta}{\partial Y^2}$$

Observe: Problem has symmetry in geometry, IC and BC about both x and y axis

Need to solve only one quadrant

Due to symmetry there is no heat flux
across X, Y axes (insulated boundaries)

IC: $\tau = 0, \quad \theta = 0$ throughout the domain

BC: $\tau > 0 \quad \theta = 1$ along sides X=1 and Y=1

$\frac{\partial \theta}{\partial Y} = 0$ along X=0 figure

$\frac{\partial \theta}{\partial X} = 0$ along Y=0

Treatment of Boundary Conditions

Types of BC (7.17)

Instead of u , $\frac{\partial u}{\partial n}$, $\frac{\partial u}{\partial s}$ or a combination may be specified at the boundary

Dirichlet condition: $u = g$

Neumann condition: $\alpha u_n + \beta u_s = g$

Mixed BC: $\alpha u_n + \beta u_s + \gamma u = g$

Where α, β, γ are constants and g is a known function.
n and s denote, respectively, the normal and tangential derivatives.

For heat transfer at the straight boundary, x = 0, (see figure), the following can be written.

$$-u_n + au = g$$

For the case shown where the boundary is at x = 0, the above equation becomes

$$-u_x + au = g$$

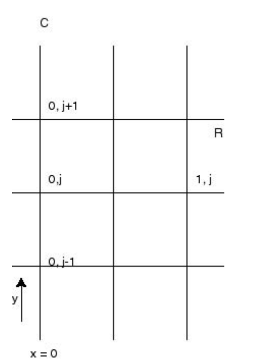

Figure 7.9 (Carnahan, Luther and Wilkes)

Consider the earlier parabolic PDE

$$u_t = u_{xx} + u_{yy}$$

u_t and u_{yy} may be obtained at the boundary as before.
Note that, when the boundary condition is given in terms of the derivatives, $u_{o,j}$ should be treated as an unknown and solved for.
An equation for i = 0 can be developed as follows.

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For u_{xx}, use Taylor series as follows to expand about (0,j)

$$u_{1,j} = u_{0,j} + u_x \Delta x + u_{xx}\frac{(\Delta x)^2}{2!} + O\left[(\Delta x)^3\right]$$

$$u_{xx} = \frac{2}{(\Delta x)^2}\left[u_{1,j} - u_{o,j} - u_x \Delta x\right] + O\left[\Delta x\right]$$

Using the BC $u_x = au - g$ we get

$$u_{xx} = \frac{2}{(\Delta x)^2}\left[u_{1,j} - (a\Delta x + 1)u_{o,j} + g\Delta x\right] + O\left[\Delta x\right]$$

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Write the corresponding equation for u_{xx} for the heat conduction problem with an insulated boundary.

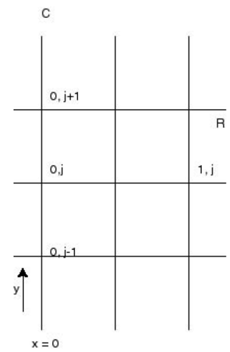

Figure 7.9 (Carnahan, Luther and Wilkes)

$$u_{xx} = \frac{2}{(\Delta x)^2}\left[u_{1,j} - u_{0,j}\right] + O\left[\Delta x\right]$$

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Final implicit form of FD approximation (2D parabolic) at point (0,j)

$$\frac{2}{(\Delta x)^2}\left[u_{1,j}^{n+1} - (a\Delta x + 1)u_{0,j}^{n+1} + g\Delta x\right] + \delta_y^2 u_{0,j}^{n+1} = \frac{u_{0,j}^{n+1} - u_{0,j}^{n}}{\Delta t}$$

Example: 1D heat conduction problem with insulated end

BC at insulated end is $\frac{\partial u}{\partial x} = 0$

Therefore from the above equation (set a=g=0)

$$u_{xx} = \frac{2}{(\Delta x)^2}\left[u_{1,j} - u_{0,j}\right] + O\left[\Delta x\right]$$

At point $(i = 0)$ equation becomes

$$\frac{2}{(\Delta x)^2}\left[u_1^{n+1} - u_0^{n+1}\right] = \frac{u_0^{n+1} - u_0^n}{\Delta t}$$

$$u_0^{n+1} - u_0^n = 2\lambda\left[u_1^{n+1} - u_0^{n+1}\right]$$

$$(1 + 2\lambda)u_0^{n+1} - 2\lambda u_1^{n+1} = u_0^n \quad \text{...........................(A)}$$

From (A)

$$b_1 = 1 + 2\lambda$$
$$c_1 = -2\lambda$$
$$\alpha_1 = u_0^n$$

Treatment of Non-linear Terms

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Non –linear PDE's

The heat conduction equation of the previous sections is linear

Fluid flow equations often have non-linear terms

Example: x-Momentum equation of 2D steady, incompressible flow

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \mu \frac{\partial^2 u}{\partial y^2}$$

Since *u* and *v* are the velocity components in x,y directions respectively the LHS terms are non-linear

Previous techniques can be adapted to solve non-linear equations

The basic approach is to linearize the equations

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In $u \frac{\partial u}{\partial x}$, if the coefficient u of $\frac{\partial u}{\partial x}$ is treated as a known quantity, then the equation becomes linear

When unsteady equations are solved u at the beginning of the time step $\left(u_{i,j}^{n}\right)$ can be used as the multiplier

For example, the first term can be discretized as

$$u_{i,j}^{n}\left(\frac{u_{i+1,j}^{n+1} - u_{i,j}^{n+1}}{\Delta x}\right)$$

Would be the fully implicit form of the first term

when we use the forward difference form for $\frac{\partial u}{\partial x}$

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Note that superscript n denotes quantities at time level t_n , which would be known from the previous solution step

Exercise: Write the same for the 2nd term

When steady state problems are solved using iterative techniques, values from the previous iteration step would be used as the multiplier u

Other non-linear forms

Consider $\frac{\partial}{\partial x}\left(D(c)\frac{\partial c}{\partial x}\right)$, the mass diffusion term in mass transfer problems.

Note D(c), the diffusion coefficient, is a function of the dependent variable, c, the concentration

If we use the model $D\left(c\right)=\alpha c+\beta$

the above term becomes

$$\frac{\partial}{\partial x}\left(D\,\frac{\partial c}{\partial x}\right)=D\left(c\right)\frac{\partial^2 c}{\partial x^2}+\alpha\left(\frac{\partial c}{\partial x}\right)^2$$

The first term on the RHS would be linearized as before using $D^n_{i,j}$ as the multiplier

To use the implicit procedure for the 2nd RHS term, it can be split as

$$\left(\frac{\partial c}{\partial x}\right)\times\left(\frac{\partial c}{\partial x}\right)$$

and treat the first half as a constant.

Note α and β are constants in the above discussion