The Advection-Diffusion Equation-I

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Computational Fluid Dynamics I

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Computational Fluid Dynamics I

Outline

Advection Diffusion equation
The cell Reynolds number

Computational Fluid Dynamics I

Methods for the advection-diffusion equation

1D Advection/diffusion equation
\[
\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = D \frac{\partial^2 f}{\partial x^2}
\]

Forward in time/centered in space (FTCS)
\[
\frac{f^{n+1}_j - f^n_j}{\Delta t} + U \frac{f^n_{j+1} - f^n_{j-1}}{2h} = D \frac{f^n_{j+1} - 2f^n_j + f^n_{j-1}}{h^2}
\]

Stability limits
\[
U \Delta t \leq 1 & \quad \frac{D \Delta t}{h^2} \leq \frac{1}{2}
\]

For high and low D

Computational Fluid Dynamics I

The Cell Reynolds number

FTCS \( O(\Delta t, h^2) \)
\[
\frac{U \Delta t}{2D} \leq 1 & \quad \frac{D \Delta t}{h^2} \leq \frac{1}{2}
\]

Upwind \( O(\Delta t, h) \)
\[
\frac{U \Delta t}{h} + \frac{D \Delta t}{h} \leq 1
\]

L-W \( O(\Delta t^2, h) \)
\[
\left( \frac{U \Delta t}{h} \right)^2 + \left( \frac{D \Delta t}{h} \right)^2 \leq 1
\]

C-N \( O(\Delta t^2, h^2) \)
Unconditionally stable
Steady state solution to the advection/diffusion equation

$$U \frac{\partial f}{\partial x} = D \frac{\partial^2 f}{\partial x^2}$$

Exact solution

$$f = \frac{\exp(R_t x/L) - 1}{\exp(R_t) - 1} \quad \text{where} \quad R_t = \frac{U}{D}$$

Numerical solution of:

$$U \frac{f_{j+1} - f_j}{2h} = D \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}$$

Centered difference approximation

$$U \frac{f_{j+1} - f_{j-1}}{2h} = D \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}$$

Upwind

$$U \frac{f_{j+1} - f_{j-1}}{h} = D \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2}$$

Solution

$$f_j = q^j$$

Substitute:

$$(R - 2)q^{j+1} + 4q^j - (R + 2)f_j = 0$$

Divide by $q^{j-1}$

$$(R - 2)q^j + 4q^j - (R + 2) = 0$$
Apply the boundary conditions

\[ f_0 = C_1 + C_2 \frac{2 + R}{2 - R} = C_1 + C_2 = 0 \]

\[ f_N = C_1 + C_2 \frac{2 + R}{2 - R} = 1 \]

The final solution is:

\[ f_j = \frac{\left( \frac{2 + R}{2 - R} \right)^j - 1}{\left( \frac{2 + R}{2 - R} \right) - 1} \]

The exact solution is:

\[ f = \frac{\exp(R_\ell x/L) - 1}{\exp(R_\ell) - 1} \quad R_\ell = \frac{UL}{D} \]

Centered differences

\[ f_j = \frac{\left( \frac{2 + R}{2 - R} \right)^j - 1}{\left( \frac{2 + R}{2 - R} \right) - 1} \]

Upwind

\[ f_j = \frac{1 - (1 + R)^j}{1 - (1 + R)} \]

Upwind

\[ U \frac{f_j - f_{j-1}}{h} = D \frac{f_{j+1} - 2f_j + f_{j-1}}{h^2} \]

or

\[ (R + 2)f_j - (R + 1)f_{j+1} - f_{j-1} = 0 \]

Try solutions

\[ f_j = q^j \]

giving

\[ q^j - (R + 2)q^j + (R + 1) = 0 \]

Solution

\[ f_j = \frac{1 - (1 + R)^j}{1 - (1 + R)} \]
When centered differencing is used for the advection/diffusion equation, oscillations may appear when the Cell Reynolds number is higher than 2. For upwinding, no oscillations appear. In most cases the oscillations are small and the cell Reynolds number is frequently allowed to be higher than 2 with relatively minor effects on the result.

\[ R = \frac{U h}{D} < 2 \]

2D example

\[
\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} + V \frac{\partial f}{\partial y} = D \left( \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} \right)
\]

Flow

\[ f = 0 \]

\[ f = 1 \]

Computations using centered differences on a 32 by 32 grid

\[ f = 0 \]

Re\(_{\text{cell}} = 3.2258 \]

D = 0.02

t = 1.5088

Re\(_{\text{cell}} = 6.4516 \]

D = 0.01

t = 1.5088

Re\(_{\text{cell}} = 12.9032 \]

D = 0.005

t = 1.5088
The Advection-Diffusion Equation-II

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Higher order in space
QUICK
Compact schemes
Conservation of energy
Higher order in time for the ψ-ω formulation

Higher order in space

Compact schemes

Centered
$$\frac{\partial f}{\partial x} \bigg|_j = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h} + O(h^4)$$

Skewed
$$\frac{\partial}{\partial x} \bigg|_j = \frac{f_{j-2} - 6f_{j-1} + 3f_j + 2f_{j+1}}{6h} + O(h^4)$$

Compact schemes
Solution of the vorticity-streamfunction equations
\[
\frac{\partial \omega}{\partial t} = \frac{\partial \omega}{\partial x} \frac{\partial \psi}{\partial y} - \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} + \sqrt{\frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2}}
\]
\[
\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = -\omega
\]

Use "compact schemes" to find O(h^4) approximations for the spatial derivatives

By a Taylor series expansion the following forth order relations between the values of f and the derivatives of f can be derived
\[
(f_{i,j})_{i+1,j} + 4(f_{i,j})_{i,j} + (f_{i,j})_{i-1,j} = \frac{3}{h^2} (f_{i+1,j} - f_{i-1,j})
\]
(1)
\[
(f_{i,j})_{i+1,j} + 4(f_{i,j})_{i,j} + (f_{i,j})_{i-1,j} = \frac{3}{h^2} (f_{i+1,j} - f_{i-1,j})
\]
(2)
\[
(f_{i,j})_{i,j+1} + 10(f_{i,j})_{i,j} + (f_{i,j})_{i,j-1} = \frac{12}{h^2} (f_{i,j+1} - 2f_{i,j} + f_{i,j-1})
\]
(3)
\[
(f_{i,j})_{i,j+1} + 10(f_{i,j})_{i,j} + (f_{i,j})_{i,j-1} = \frac{12}{h^2} (f_{i,j+1} - 2f_{i,j} + f_{i,j-1})
\]
(4)

The vorticity-streamfunction equations at grid point i,j are
\[
\left(\frac{\partial \psi}{\partial y}\right)_{i,j} = \left(\frac{\partial \omega}{\partial x}\right)_{i,j} + \left(\frac{\partial \omega}{\partial y}\right)_{i,j} + \left(\frac{\partial^2 \omega}{\partial x^2}\right)_{i,j} + \left(\frac{\partial^2 \omega}{\partial y^2}\right)_{i,j}
\]
(5)
\[
\left(\frac{\partial^2 \psi}{\partial x^2}\right)_{i,j} + \left(\frac{\partial^2 \psi}{\partial y^2}\right)_{i,j} = -\omega_{i,j}
\]
(6)

To find the time derivative, we need

\[\psi', \psi', \psi', \psi', \omega', \omega, \omega, \omega, \omega, \omega\]

1. Given the vorticity, \( \omega \), we solve tridiagonal equations (1-4) for \( \omega_x, \omega_y, \omega_{xx}, \omega_{yy} \)
2. For \( \psi \) use (3) and (4) plus the elliptic equation for the streamfunction (6) for \( \psi' = \psi' = \psi \)
3. Then use 1 and 2 for (tridiagonal systems) \( \psi' = \psi' \)
4. Everything on the right hand side of (5) is now known to O(h^4) accuracy and can be found

The main advantage of compact schemes is that it is somewhat easier to implement boundary conditions than for high order schemes that use a broad stencil

Higher order upwind QUICK
Essentially Non-Oscillating (ENO) scheme of Shu and Osher

1. Construct left and right slopes by connecting the average values in adjacent cells
2. Select the downstream flux by using the smaller slope

\[ f_{j+1/2} = \begin{cases} 
    f_j + \frac{1}{2} \min \left( \Delta f^+, \Delta f^- \right), & \text{if } \frac{1}{2} (u_j + u_{j+1}) > 0 \\
    f_j - \frac{1}{2} \min \left( \Delta f^+, \Delta f^- \right), & \text{if } \frac{1}{2} (u_j + u_{j+1}) < 0 
\end{cases} \]
Second order ENO scheme for the linear advection equation
\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0
\]
\[
f_j = \begin{cases} 
\hat{f}_j - \Delta f \left( f_{j1/2} - f_{j-1/2} \right) & \text{if } \frac{1}{2}(u_j + u_{j+1}) > 0 \\
\hat{f}_j + \frac{1}{2} \Delta f \left( f_{j1/2} + f_{j-1/2} \right) & \text{if } \frac{1}{2}(u_j + u_{j+1}) < 0
\end{cases}
\]
\[
f_{j1/2} = \begin{cases} 
\hat{f}_j & \text{if } f_j = f_j \left( f_{j1/2} - f_{j-1/2} \right) \\
\hat{f}_j & \text{if } f_j = f_j \left( f_{j1/2} + f_{j-1/2} \right)
\end{cases}
\]

Conservation of kinetic energy

Consider two different discretizations of the nonlinear term
\[
\frac{df}{dt} = -f \frac{df}{dx} = -\frac{1}{2} \left( f_{j-1/2} - f_{j+1/2} \right)
\]
and
\[
\frac{df}{dt} = -\frac{1}{2} \left( f_{j-1/2} - f_{j+1/2} \right)
\]
Both conserve \( f \)

Is \( f \) conserved?
Write out the terms for the kinetic energy

\[ \frac{df}{dt} = -\frac{1}{2h} \left[ \alpha f_j(f_{j+1} - f_j) - \frac{1 - \alpha}{2} f_j f_j \right] \]

Write out the terms for the kinetic energy

\[ \int \frac{d\psi^2}{dx} dx = -\frac{1}{2} \sum \left[ \alpha f_j(f_{j+1} - f_j) - \frac{1 - \alpha}{2} f_j f_j \right] \]

\[ = \ldots + \alpha f_j^2(f_{j+1} - f_j) + \frac{1 - \alpha}{2} f_j f_j + \alpha f_j(f_{j+1} - f_j) - \frac{1 - \alpha}{2} f_j f_j + \ldots = 0 \]

The same idea is used in Arakawa’s scheme (JCP 119, 1966)

Consider the vorticity advection equation

\[ \frac{\partial \omega}{\partial t} + u \cdot \nabla \omega = 0 \]

Rewrite the nonlinear terms to introduce the Jacobian

\[ u \cdot \nabla \omega = -\frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial x} + \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} = J(\psi, \omega) \]

\[ \frac{\partial \omega}{\partial x} + J(\psi, \omega) = 0 \]

we also have

\[ J(\psi, \omega) = -J(\omega, \psi) \]

since

\[ J(\psi, \omega) = \frac{\partial \psi}{\partial x} \frac{\partial \omega}{\partial y} - \frac{\partial \psi}{\partial y} \frac{\partial \omega}{\partial x} = \left( \frac{\partial \omega}{\partial x} \frac{\partial \psi}{\partial y} - \frac{\partial \omega}{\partial y} \frac{\partial \psi}{\partial x} \right) \]

Discretization of the different forms of the Jacobian give schemes with slightly different conservation properties

\[ f_{i,j} = \frac{1}{4h^2} \left[ \begin{array}{c} \alpha_{i+1,j} - \alpha_{i,j} \\ \alpha_{i,j} - \alpha_{i-1,j} \end{array} \right] (\psi_{i+1,j} - \psi_{i,j}) \]

\[ J_{i,j} = \frac{1}{4h^2} \left[ \begin{array}{c} \omega_{i+1,j} \\ \omega_{i,j} \end{array} \right] (\psi_{i+1,j} - \psi_{i,j}) - \omega_{i,j} (\psi_{i+1,j} - \psi_{i,j}) \]

\[ J_{i,j} = \frac{1}{4h^2} \left[ \begin{array}{c} \omega_{i+1,j} - \omega_{i-1,j} \\ \omega_{i+1,j} - \omega_{i,j} \end{array} \right] (\psi_{i+1,j} - \psi_{i,j}) \]

\[ J_{i,j} = \frac{1}{4h^2} \left[ \begin{array}{c} \psi_{i+1,j} - \psi_{i,j} \\ \psi_{i,j} \end{array} \right] (\omega_{i+1,j} - \omega_{i-1,j}) + \psi_{i+1,j} (\omega_{i+1,j} - \omega_{i+1,j}) \]

\[ + \psi_{i,j} (\omega_{i,j} - \omega_{i+1,j}) - \psi_{i,j} (\omega_{i,j} - \omega_{i+1,j}) \]
Runge Kutta methods: take intermediate steps

2nd order Runge-Kutta

\[
\begin{align*}
\nabla^2 \psi_j^i &= -\omega_j^i \\
\hat{\omega}_j^i &= \omega_j^i + \frac{\Delta t}{2} \left( -J_j^i + \nabla^2 \omega_j^i \right) \\
\nabla^2 \psi_j^i &= -\omega_j^i \\
\hat{\omega}_j^i &= \omega_j^i + \Delta t \left( -J_j^i + \nabla^2 \omega_j^i \right)
\end{align*}
\]

Half step

Final step

Higher order in time for the vorticity-streamfunction formulation

Due to the relatively straightforward coupling between the elliptic equation for the streamfunction and the vorticity advection-diffusion equation, the algorithms discussed already can be used with ease.

Arakawa showed that

\[ J_{ij}^1 = \frac{1}{3} (J_{ij}^0 + J_{ij}^1 + J_{ij}^0) \]

Conserves both the vorticity and the kinetic energy

Arakawa also presented a fourth order scheme with the same properties

Leapfrog

\[
\frac{\omega_{ij}^{n+1} - \omega_{ij}^n}{2\Delta t} = -J_{ij}^n + \nabla^2 \omega_{ij}^n
\]

Adams-Bashford/Crank-Nicholson

\[
\frac{\omega_{ij}^{n+1} - \omega_{ij}^n}{\Delta t} = \frac{1}{2} \left( 3J_{ij}^n - J_{ij}^{n-1} \right) + \frac{\nu}{2} \left( \nabla^2 \omega_{ij}^n + \nabla^2 \omega_{ij}^{n-1} \right)
\]

Predictor-corrector

\[
\frac{\hat{\omega}_{ij}^n - \omega_{ij}^n}{\Delta t} = -J_{ij}^n + \nabla^2 \omega_{ij}^n
\]

\[
\frac{\hat{\omega}_{ij}^{n+1} - \omega_{ij}^n}{\Delta t} = -\frac{1}{2} \left( J_{ij}^n + J_{ij}^{n-1} \right) + \frac{\nu}{2} \left( \nabla^2 \omega_{ij}^n + \nabla^2 \omega_{ij}^{n-1} \right)
\]

4th order Runge-Kutta method

\[
\begin{align*}
\nabla^2 \psi_j^{i+1} &= -\omega_j^{i+1} \\
\hat{\omega}_j^{i+1} &= \omega_j^{i+1} + \frac{\Delta t}{2} \left( -J_j^{i+1} + \nabla^2 \omega_j^{i+1} \right) \\
\nabla^2 \psi_j^{i+1/2} &= \hat{\omega}_j^{i+1} \\
\hat{\omega}_j^{i+1/2} &= \omega_j^{i+1/2} + \frac{\Delta t}{2} \left( -J_j^{i+1/2} + \nabla^2 \omega_j^{i+1/2} \right) \\
\nabla^2 \psi_j^{i+1/2} &= -\omega_j^{i+1/2} \\
\hat{\omega}_j^{i-1} &= \omega_j^{i-1} + \Delta t \left( J_j^{i+1/2} + \nabla^2 \omega_j^{i+1/2} \right) \\
\nabla^2 \psi_j^{i-1} &= \hat{\omega}_j^{i-1} \\
\hat{\omega}_j^{i} &= \omega_j^{i} + \Delta t \left( J_j^{i+1/2} + \nabla^2 \omega_j^{i+1/2} \right)
\end{align*}
\]

First half step

Second half step

Predicted final value
Computational Fluid Dynamics I

4th order Runge-Kutta method (continued)

\[ \nabla_h^2 \psi_{i,j}^{n+1} = -\tilde{\omega}_{i,j}^{n+1} \]

\[ \tilde{\omega}_{i,j}^{n+1} = \tilde{\omega}_{i,j}^{n} + \frac{\Delta t}{6} \left( -J_{i,j}^{n} - 2J_{i,j}^{n+1/2} - 2J_{i,j}^{n+1} - \tilde{J}_{i,j}^{n+1} \right) \]

\[ + \nu \nabla_h^2 \tilde{\omega}_{i,j}^{n} + 2\nu \nabla_h^2 \tilde{\omega}_{i,j}^{n+1/2} + 2\nu \nabla_h^2 \tilde{\omega}_{i,j}^{n+1} + \nu \nabla_h^2 \tilde{\omega}_{i,j}^{n+1} \]

corrected final value

Generating higher order methods for the Navier-Stokes equations in the curl/circulation/ streamfunction form is relatively straightforward and any method developed for the advection diffusion equation can be used without much difficulty.