The Advection-Diffusion equation

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The Navier-Stokes equations contain three equation types that have their own characteristic behavior. Depending on the governing parameters, one behavior can be dominant. The different equation types require different solution techniques. For inviscid compressible flows, only the hyperbolic part survives.

Computational Fluid Dynamics

1D Advection/diffusion equation

\[ \frac{df}{dt} + U \frac{df}{dx} = D \frac{d^2f}{dx^2} \]

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:

- \[ \frac{U \Delta t}{2D} \leq 1 \]
- \[ \frac{D \Delta x^2}{h^2} \leq \frac{1}{2} \]
- \[ R = \frac{UL}{D} \]
- \[ \Delta = \frac{2D}{U} \]
- \[ \Delta = \frac{h^2}{2D} \]

\[ \Delta t \to 0 \quad \text{For high and low D} \]

Steady state solution to the advection/diffusion equation

\[ U \frac{df}{dx} = D \frac{d^2f}{dx^2} \]

\[ f = 0 \quad \text{at} \quad x = 0 \]
\[ f = 1 \quad \text{at} \quad x = L \]

Exact solution

\[ f = \frac{\exp(R_L x/L) - 1}{\exp(R_L) - 1} \quad R_L = \frac{UL}{D} \]
Computational Fluid Dynamics

The Cell Reynolds number

Centered difference approximation

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

Rearrange:

\[ \frac{Uh^2}{2hD}(f_{j+1} - f_{j-1}) = f_{j+1} - 2f_j + f_{j-1} \]

Rearrange:

\[ (R - 2)f_{j+1} + 4f_j - (R + 2)f_{j-1} = 0 \]

Where: \( R = \frac{Uh}{D} \)

Solving for \( q \) gives two solutions:

\[ q_1 = 1 \quad \text{and} \quad q_2 = \frac{2 + R}{2 - R} \]

The general solution is:

\[ f_j = C_1 q_1^j + C_2 q_2^j \]

or

\[ f_j = C_1 + C_2 \left( \frac{2 + R}{2 - R} \right)^j \]

Apply the boundary conditions

\[ f_0 = C_1 + C_2 \left( \frac{2 + R}{2 - R} \right)^0 = C_1 + C_2 = 0 \]

\[ f_N = C_1 + C_2 \left( \frac{2 + R}{2 - R} \right)^N = 1 \]

The final solution is:

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

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

- \( f = 0 \) (Flow)
- \( f = 1 \) (Computations using centered differences on a 32 by 32 grid)
- \( f = 0 \)

Computational Fluid Dynamics

\( D = 0.02 \)
\( t = 1.5088 \)
\( \text{Re}_{\text{cell}} = 3.2258 \)

\( D = 0.01 \)
\( t = 1.5088 \)
\( \text{Re}_{\text{cell}} = 6.4516 \)

\( D = 0.005 \)
\( t = 1.5088 \)
\( \text{Re}_{\text{cell}} = 12.9032 \)

Stability in terms of Fluxes
Consider the following initial conditions:

$$f_{j-1}^i, f_j^i, f_{j+1}^i$$

During one time step, $U \Delta t/h$ of $f$ flows into cell $j$, increasing the average value of $f$ by $U \Delta t/h$.

If $U \Delta t/h > 1$, the average value of $f$ in cell $j$ will be larger than in cell $j-1$. In the next step, $f$ will flow out of cell $j$ in both directions, creating a larger negative value of $f$. Taking a third step will result in an even larger positive value, and so on until the compute encounters a NaN (Not a Number).
By considering the fluxes, it is easy to see why the centered difference approximation is always unstable.

Consider the following initial conditions:

\[ F_{j+1/2} = \frac{U}{2} (f^+_{j+1} + f^+_{j}) = 1.0 \quad F_{j-1/2} = \frac{U}{2} (f^-_{j} + f^-_{j+1}) = 0.5 \]

\[ f_{j+1} = f_j - \frac{\Delta t}{h} (F_{j+1/2} - F_{j-1/2}) = 1.0 - 0.5(0.5 - 1) = 1.25 \]

So cell \( j \) will overflow immediately!

**Advection by Higher Order Methods**

For the advection terms, the methods described for hyperbolic equations, including ENO, can all be applied, yielding stable and robust methods that can be “forgiving” for low resolution.

QUICK, where a third order upstream differencing is used is also popular.

Use to solve:

\[ \frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial f}{\partial x} = D \frac{\partial^2 f}{\partial x^2} \]

At \( s = 5/2 \),

\[ f_{s/2} = (1/8)(3f_1 + 6f_2 - f_3) \]

\[ \frac{\partial f}{\partial x} = \frac{1}{h} \left( f_{s+1/2} - f_{s-1/2} \right) \]

\[ = \frac{1}{64h} \left( \left[ 3f_{s+1} + 6f_s - f_{s-1} \right]^3 - \left[ 3f_s + 6f_{s-1} - f_{s-2} \right]^3 \right) \]
Second order ENO scheme for the linear advection equation

\[
\frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} = 0
\]

\[
f_j^* = f_j - \frac{\Delta t}{2} \left( f_{i+1/2} - f_{i-1/2} \right)
\]

\[
f_j^{**} = f_j^* - \frac{\Delta t}{12} \left( f_{i+1/2} - f_{i-1/2} \right) + \frac{u}{2} \left( f_{i+1/2} - f_{i-1/2} \right)
\]

\[
f_{i+1/2} = \begin{cases} 
  f_i + \frac{1}{3} \min(\Delta f_i, \Delta f_{i+1}), & \text{if } u_j + u_{j+1} > 0 \\
  f_i - \frac{1}{3} \min(\Delta f_{i+1}, \Delta f_i), & \text{if } u_j + u_{j+1} < 0 
\end{cases}
\]

\[
\Delta f_i = f_{i+1} - f_i, \quad \Delta f_{i+1} = f_{i+1} - f_{i+1/2}
\]

Higher order finite difference approximations

The simplest approach is to use more points:

\[
\begin{align*}
& f_i - 2h, f_i, f_{i+2h}, f_{i+h}, f_{i+3h}, f_{i+4h} \\
& \frac{h}{12} h
\end{align*}
\]
Compact schemes

By a Taylor series expansion the following fourth order relations between the values of $f$ and the derivatives of $f$ can be derived:

\[ f_i = f_{i+1} + \frac{\partial f}{\partial x} \Delta x + \frac{\partial^2 f}{\partial x^2} \frac{\Delta x^2}{2} + \frac{\partial^3 f}{\partial x^3} \frac{\Delta x^3}{6} + \frac{\partial^4 f}{\partial x^4} \frac{\Delta x^4}{24} + O(\Delta x^4) \]  
(1)

\[ f_i = f_{i-1} - \frac{\partial f}{\partial x} \Delta x + \frac{\partial^2 f}{\partial x^2} \frac{\Delta x^2}{2} - \frac{\partial^3 f}{\partial x^3} \frac{\Delta x^3}{6} + \frac{\partial^4 f}{\partial x^4} \frac{\Delta x^4}{24} + O(\Delta x^4) \]  
(2)

Adding $f_i + f_{i-1} = 2f_i + \frac{\partial f}{\partial x} \Delta x + \frac{\partial^2 f}{\partial x^2} \frac{\Delta x^2}{12} + O(\Delta x^4)$

Taking the second derivative:

\[ f_i + f_{i-1} = 2f_i + \frac{\partial f}{\partial x} \Delta x + \frac{\partial^2 f}{\partial x^2} \frac{\Delta x^2}{12} + O(\Delta x^4) \]  
(3)

Eliminating the fourth derivative:

\[ f_i + 10f_i + f_{i-1} = \frac{12}{\Delta x^2} (f_i - 2f_{i+1} + f_{i-1}) + O(\Delta x^4) \]  
(4)

To solve the nonlinear advection-diffusion equation

\[ \frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} - \nu \frac{\partial^2 f}{\partial x^2} = 0 \]

we first solve the first and second derivatives using the expressions derived above:

\[ \frac{\partial f}{\partial t} + u \frac{\partial f}{\partial x} - \nu \frac{\partial^2 f}{\partial x^2} = \frac{1}{\Delta t} \left( f_{i+1} - f_{i-1} \right) + O(\Delta t) \]

\[ \frac{\partial^2 f}{\partial x^2} = \frac{1}{\Delta x^2} \left( f_{i+1} - 2f_i + f_{i-1} \right) + O(\Delta x^4) \]

And use the values to compute the RHS. The time integration is then done using a high order time integration method.

The standard way to obtain higher order approximations to derivatives is to include more points. This can lead to very wide stencils and near boundaries this requires a large number of "ghost" points outside the boundary. This can be overcome by "compact" schemes, where we derive expressions relating the derivatives at neighboring points to each other and the function values.

A large number of advanced numerical methods have been developed for hyperbolic, parabolic and elliptic equations. These methods can be applied directly to the Navier-Stokes equations, although the structure of the equations generally requires us to pay close attention in which order the solution proceeds.