Computational Fluid Dynamics

Lecture 7
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Classical Methods

Discontinuous solutions

Entropy conditions

Shock speed

Conservative discretization

Classical Methods for Hyperbolic Equations

The wave equation:

$$\frac{\partial^2 f}{\partial t^2} - c^2 \frac{\partial^2 f}{\partial x^2} = 0$$

Write as:

$$\frac{\partial u}{\partial t} - c^2 \frac{\partial v}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} - \frac{\partial u}{\partial x} = 0$$

In general:

$$\begin{bmatrix} \dfrac{\partial u}{\partial t} \\ \dfrac{\partial v}{\partial t} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} \dfrac{\partial u}{\partial x} \\ \dfrac{\partial v}{\partial x} \end{bmatrix} = 0$$

Most of the issues involved can be addressed by examining:

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = 0$$

Forward in Time, Centered in Space (FTCS) and Upwind

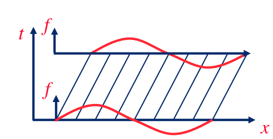
We will start by examining the linear advection equation:

$$\frac{\partial f}{\partial t} + U \frac{\partial f}{\partial x} = 0$$

The characteristic for this equation are:

$$\frac{dx}{dt} = U; \quad \frac{df}{dt} = 0;$$

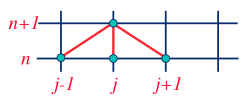
Showing that the initial conditions are simply advected by a constant velocity U



$$\frac{\partial f}{\partial t}+U\frac{\partial f}{\partial x}=0$$

A simple forward in time, centered in space discretization yields

$$f_j^{n+1}=f_j^n-\frac{\Delta t}{2h}U(f_{j+1}^n-f_{j-1}^n)$$

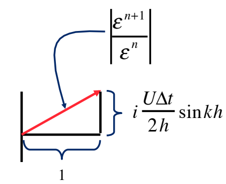


Computational Fluid Dynamics
Methods for Advection

This scheme is O(Δt, h²) accurate, but a stability analysis shows that the error grows as

$$\frac{\varepsilon^{n+1}}{\varepsilon^n}=1-i\frac{U\Delta t}{2h}\sin kh$$

Since the amplification factor has the form 1+*i*() the absolute value of this complex number is always larger than unity and the method is unconditionally unstable for this case.



Computational Fluid Dynamics
Methods for Advection

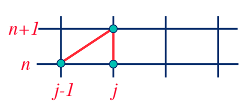
Another scheme for

$$\frac{\partial f}{\partial t}+U\frac{\partial f}{\partial x}=0$$

A simple forward in time but "upwind" in space discretization yields

$$f_j^{n+1}=f_j^n-\frac{\Delta t}{h}U(f_j^n-f_{j-1}^n)$$

Flow direction



This scheme is O(Δt, h) accurate.

Computational Fluid Dynamics
Methods for Advection

To examine the stability we use the von Neuman's method:

The evolution of the error is governed by:

$$\frac{\varepsilon_j^{n+1}-\varepsilon_j^n}{\Delta t}+\frac{U}{h}(\varepsilon_j^n-\varepsilon_{j-1}^n)=0$$

Write the error as: $\varepsilon_j^n=\varepsilon^n e^{ikx_j}$

$$\frac{\varepsilon^{n+1}-\varepsilon^n}{\Delta t}+U\frac{\varepsilon^n}{h}(1-e^{-ikh})=0 \longrightarrow \frac{\varepsilon^{n+1}}{\varepsilon^n}=1-\frac{U\Delta t}{h}(1-e^{-ikh})$$

Amplification factor

$$G=\frac{\varepsilon^{n+1}}{\varepsilon^n}=1-\lambda(1-e^{-ikh}),\qquad \lambda=\frac{U\Delta t}{h}$$

Or: $G=1-\lambda+\lambda e^{-ikh}$ Need to find when $|G|<1$

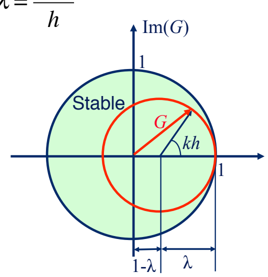
Computational Fluid Dynamics
Methods for Advection

Graphically:

$$G=1-\lambda+\lambda e^{-ikh},\qquad \lambda=\frac{U\Delta t}{h}$$

Stability condition: λ<1

$$\boxed{\frac{U\Delta t}{h}\le 1}$$



This restriction was first derived by Courant, Fredrik, and Levy in 1932, and is usually called the Courant condition, or the CFL condition.

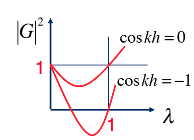
Computational Fluid Dynamics
Methods for Advection

Another way: Find the absolute value of the amplification factor

$$G=1-\lambda+\lambda e^{-ikh}=1-\lambda+\lambda\cos kh-i\lambda\sin kh$$

$$\begin{aligned}|G|^2&=(1-\lambda+\lambda\cos kh)^2+\lambda^2\sin^2 kh\\&=(1-\lambda)^2+2(1-\lambda)\lambda\cos kh+\lambda^2\cos^2 kh+\lambda^2\sin^2 kh\\&=(1-\lambda)^2+2(1-\lambda)\lambda\cos kh+\lambda^2\\&=1-2\lambda+2\lambda^2+2(1-\lambda)\lambda\cos kh\end{aligned}$$

$$\begin{aligned}|G|^2&=1-2\lambda(1-\lambda) && \text{if } \cos kh=0\\|G|^2&=1 && \text{if } \cos kh=1\\|G|^2&=1-\lambda(4-3\lambda) && \text{if } \cos kh=-1\end{aligned}$$

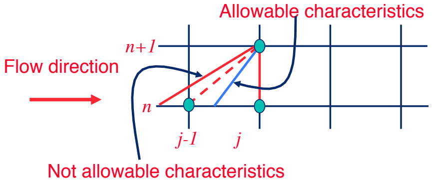


$$\longrightarrow\ |G|^2\le 1 \quad \text{if} \quad \lambda\le 1$$

Computational Fluid Dynamics
Methods for Advection

The CFL condition implies that a signal has to travel less than one grid spacing in one time step

$$U\Delta t \le h$$

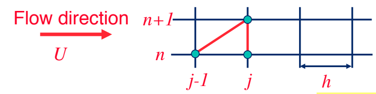


Computational Fluid Dynamics
Methods for Advection

The Upwind Scheme

For the linear advection equation: $\frac{\partial f}{\partial t} + U\frac{\partial f}{\partial x} = 0$

$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h}U(f_j^n - f_{j-1}^n)$$

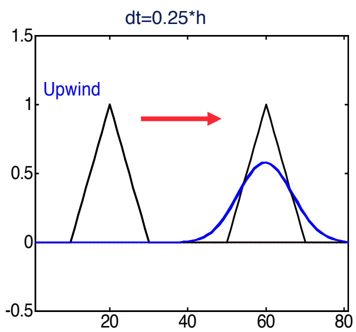


O(Δt, h) accurate.

$$\frac{U\Delta t}{h} \le 1$$

Computational Fluid Dynamics
Methods for Advection

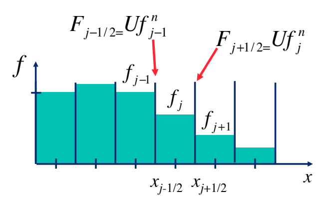
Although the upwind method is exceptionally robust, its low accuracy in space and time makes it unsuitable for most serious computations



Computational Fluid Dynamics
Methods for Advection

Finite Volume point of view:

$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h}(F_{j+1/2}^n - F_{j-1/2}^n) = f_j^n - \frac{\Delta t}{h}U(f_j^n - f_{j-1}^n)$$



Computational Fluid Dynamics

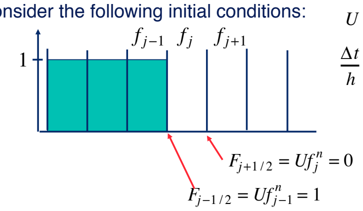
Stability in terms of Fluxes for the upwind scheme

Computational Fluid Dynamics
Stability in terms of fluxes

Consider the following initial conditions:

$$U = 1$$

$$\frac{\Delta t}{h} = 1.5 \cdot U = 1.5$$

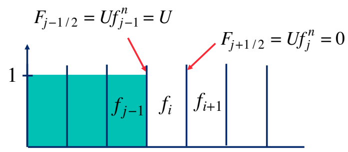


During one time step, $U\Delta t$ of f flows into cell j, increasing the average value of f by $U\Delta t/h$.

Computational Fluid Dynamics
Stability in terms of fluxes

$\frac{\Delta t}{h} = 1.5 \cdot U = 1.5$

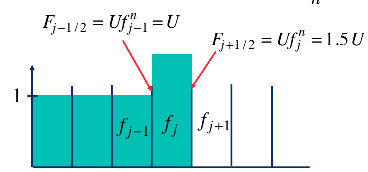
Consider the following initial conditions:



$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h}(F_{j+1/2}^n - F_{j-1/2}^n) = 0 - 1.5(0-1) = 1.5$$

Computational Fluid Dynamics
Stability in terms of fluxes

$\frac{\Delta t}{h} = 1.5 \cdot U = 1.5$

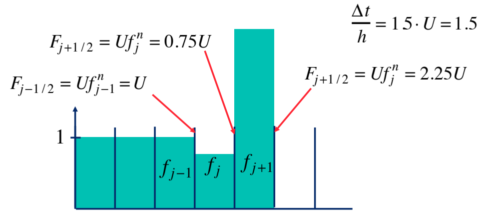


$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h}(F_{j+1/2}^n - F_{j-1/2}^n) = 0 - 1.5(1.5-1) = 0.75$$

$$f_{j+1}^{n+1} = f_{j+1}^n - \frac{\Delta t}{h}(F_{j+3/2}^n - F_{j+1/2}^n) = 0 - 1.5(0 - 1.5) = 2.25$$

Computational Fluid Dynamics
Stability in terms of fluxes

$\frac{\Delta t}{h} = 1.5 \cdot U = 1.5$



Taking a third step will result in an even larger positive value, and so on until the compute encounters a NaN (Not a Number).

Computational Fluid Dynamics
Stability in terms of fluxes

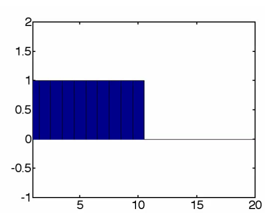
If $U\Delta t/h > 1$, the average value of f in cell j will be larger than in cell j-1. In the next step, f will flow out of cell j in both directions, creating a larger negative value of f. Taking a third step will result in an even larger positive value, and so on until the compute encounters a NaN (Not a Number).

Computational Fluid Dynamics
Stability in terms of fluxes

MOVIE FROM MATLAB

```
% one-dimensional advection by first order upwind.
n=80; nstep=100; dt=0.0125; length=2.0;
h=length/(n-1);y=zeros(n,1);f=zeros(n,1);f(1)=1.0;

for m=1:nstep,m
   hold off, plot(f); axis([1, n, -0.5, 1.5]);
   pause(0.01);
   y=f;
   for i=2:n-1,
      f(i)=y(i)-(dt/h)*(y(i)-y(i-1)); %upwind
    end;
end;
```



Computational Fluid Dynamics

Generalized Upwind Scheme (for both $U > 0$ and $U < 0$)

$$f_j^{n+1} = f_j^n - \frac{U\Delta t}{h}(f_j^n - f_{j-1}^n), \; U > 0$$

$$f_j^{n+1} = f_j^n - \frac{U\Delta t}{h}(f_{j+1}^n - f_j^n), \; U < 0$$

Define: $U^+ = \frac{1}{2}(U + |U|), \; U^- = \frac{1}{2}(U - |U|)$

The two cases can be combined into a single expression:

$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h}\left[U^+(f_j^n - f_{j-1}^n) + U^-(f_{j+1}^n - f_j^n)\right]$$

Or, substituting U^+, U^-

$$f_j^{n+1} = f_j^n - U\frac{\Delta t}{2h}(f_{j+1}^n - f_{j-1}^n) + \frac{|U|\Delta t}{2h}(f_{j+1}^n - 2f_j^n + f_{j-1}^n)$$

central difference + numerical viscosity

$D_{num} = \frac{|U|h}{2}$

Computational Fluid Dynamics

Other First Order Schemes

Computational Fluid Dynamics
Methods for Advection

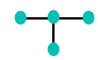
Implicit (Backward Euler) Method

$$\frac{f_j^{n+1}-f_j^n}{\Delta t}+\frac{U}{2h}\left(f_{j+1}^{n+1}-f_{j-1}^{n+1}\right)=0$$

- Unconditionally stable
- 1st order in time, 2nd order in space
- Forms a tri-diagonal matrix (Thomas algorithm)

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

$$a_j f_{j+1}^{n+1}+d_j f_j^{n+1}+b_j f_{j-1}^{n+1}=C_j$$



Computational Fluid Dynamics
Methods for Advection

Lax-Fredrichs method

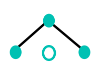
Start with the unstable centered difference approximation

$$\frac{f_j^{n+1}-f_j^n}{\Delta t}+\frac{U}{2h}\left(f_{j+1}^n-f_{j-1}^n\right)=0$$

Replace the old value by

$$f_j^n \to \tfrac{1}{2}\left(f_{j+1}^n+f_{j-1}^n\right)$$

Resulting in



$$\frac{f_j^{n+1}-\frac{1}{2}\left(f_{j+1}^n+f_{j-1}^n\right)}{\Delta t}+\frac{U}{2h}\left(f_{j+1}^n-f_{j-1}^n\right)=0$$

Computational Fluid Dynamics
Methods for Advection

Lax-Fredrichs method

- stable for $\lambda < 1$
- 1st order in time and space
- Conditionally consistent, but!

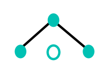
$$\lambda=\frac{U\Delta t}{h}$$

$$\frac{h}{\lambda}=\frac{h^2}{U\Delta t}$$

Error term:

$$\frac{Uh}{2}\left(\frac{1}{\lambda}-\lambda\right)f_{xx}+\frac{Uh^2}{3}\left(1-\lambda^2\right)f_{xxx}$$

$$\frac{1}{2}\left(\frac{h^2}{\Delta t}-U\Delta t\right)f_{xx}+\frac{1}{3}\left(Uh^2-U^3\Delta t^2\right)f_{xxx}$$



If we assume that $\Delta t \sim h$ then we have

$O(\Delta t, h)$

Used as a starting point for higher order methods

Computational Fluid Dynamics

Second Order Schemes

Computational Fluid Dynamics
Methods for Advection

Leap Frog Method

The simplest stable second-order accurate (in time) method:

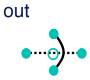
$$\frac{\partial f}{\partial t}=\frac{f_j^{n+1}-f_j^{n-1}}{2\Delta t}+O(\Delta t^2)$$

$$f_j^{n+1}=f_j^{n-1}-\frac{U\Delta t}{h}\left(f_{j+1}^n-f_{j-1}^n\right)$$

$$\lambda=\frac{U\Delta t}{h}$$

Modified equation
$$\frac{\partial f}{\partial t}+U\frac{\partial f}{\partial x}=\frac{Uh^2}{6}\left(\lambda^2-1\right)f_{xxx}+\cdots$$

- Stable for $|\lambda|<1$
- Dispersive (no dissipation) – error will not damp out
- Initial conditions at two time levels
- Oscillatory solution in time (alternating)



Lax-Wendroff's Method (LW-I)

First expand the solution in time

$$f(t+\Delta t) = f(t) + \frac{\partial f}{\partial t}\Delta t + \frac{\partial^2 f}{\partial t^2}\frac{\Delta t^2}{2} + \frac{\partial^3 f}{\partial t^3}\frac{\Delta t^3}{6} + \cdots$$

Then use the original equation to rewrite the time derivatives

$$\frac{\partial f}{\partial t} = -U\frac{\partial f}{\partial x}$$

$$\frac{\partial^2 f}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial f}{\partial t}\right) = -\frac{\partial}{\partial t}\left(U\frac{\partial f}{\partial x}\right) = -U\frac{\partial}{\partial x}\frac{\partial f}{\partial t} = U^2\frac{\partial^2 f}{\partial x^2}$$

Computational Fluid Dynamics
Methods for Advection

Substituting

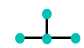
$$f(t+\Delta t) = f(t) - U\frac{\partial f}{\partial x}\Delta t + U^2\frac{\partial^2 f}{\partial x^2}\frac{\Delta t^2}{2} + O(\Delta t^3)$$

Using central differences for the spatial derivatives

$$f_j^{n+1} = f_j^n - \frac{U\Delta t}{2h}\left(f_{j+1}^n - f_{j-1}^n\right) + \frac{U^2\Delta t^2}{2h^2}\left(f_{j+1}^n - 2f_j^n + f_{j-1}^n\right)$$

2nd order accurate in space and time

Stable for $\frac{U\Delta t}{h} < 1$



Computational Fluid Dynamics
Methods for Advection

Two-Step Lax-Wendroff's Method (LW-II)

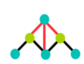
LW-I into two steps:

$$\frac{f_{j+1/2}^{n+1/2} - (f_{j+1}^n + f_j^n)/2}{\Delta t/2} + U\frac{f_{j+1}^n - f_j^n}{h} = 0 \qquad \text{Step 1 (Lax)}$$

$$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U\frac{f_{j+1/2}^{n+1/2} - f_{j-1/2}^{n+1/2}}{h} = 0 \qquad \text{Step 2 (Leapfrog)}$$

- Stable for $U\Delta t/h < 1$
- Second order accurate in time and space

For the linear equations, LW-II is identical to LW-I



Computational Fluid Dynamics
Methods for Advection

MacCormack Method

Similar to LW-II, without $j+1/2,\ j-1/2$

$$f_j' = f_j^n - U\frac{\Delta t}{h}\left(f_{j+1}^n - f_j^n\right) \qquad \text{Predictor}$$

$$f_j^{n+1} = \frac{1}{2}\left[f_j^n + f_j' - U\frac{\Delta t}{h}\left(f_j' - f_{j-1}'\right)\right] \qquad \text{Corrector}$$

- A fractional step method
  - Predictor: forward differencing
  - Corrector: backward differencing
- For linear problems, accuracy and stability properties are identical to LW-I.

Computational Fluid Dynamics
Methods for Advection

Second-Order Upwind Method

Warming and Beam (1975) – Upwind for both steps

$$f_j' = f_j^n - U\frac{\Delta t}{h}\left(f_j^n - f_{j-1}^n\right) \qquad \text{Predictor}$$

Corrector

$$f_j^{n+1} = \frac{1}{2}\left[f_j^n + f_j' - U\frac{\Delta t}{h}\left(f_j' - f_{j-1}'\right) - U\frac{\Delta t}{h}\left(f_j^n - 2f_{j-1}^n + f_{j-2}^n\right)\right]$$

Combining the two:

$$f_j^{n+1} = f_j^n - \lambda\left(f_j^n - f_{j-1}^n\right) + \frac{1}{2}\lambda(\lambda-1)\left(f_j^n - 2f_{j-1}^n + f_{j-2}^n\right)$$

- Stable if $0 \le \lambda \le 2$
- Second-order accurate in time and space

Computational Fluid Dynamics
Methods for Advection

The one-step Lax-Wendroff is not easily extended to non-linear or multi-dimensional problems. The split version is.

In the Lax-Wendroff and the MacCormack methods the spatial and the temporal discretization are not independent.

Other methods have been developed where the time integration is independent of the spatial discretization, such as the Beam-Warming and various Runge-Kutta methods

Computational Fluid Dynamics
Summary

$$f_t + U f_x = 0$$

FTCS	$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{f_{j+1}^n - f_{j-1}^n}{2h} = 0$	$-\Delta t \frac{U^2}{2} f_{xx} - \frac{Uh^2}{6}(1 + 2\lambda^2) f_{xxx}$	Unconditionally Unstable
Upwind	$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{f_j^n - f_{j-1}^n}{h} = 0$	$\frac{Uh}{2}(1-\lambda) f_{xx} - \frac{Uh^2}{6}(2\lambda^2 - 3\lambda + 1) f_{xxx}$	Stable for $\lambda \le 1$
Implicit	$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{(f_{j+1}^{n+1} - f_{j-1}^{n+1})}{2h} = 0$	$\frac{U^2 \Delta t}{2} f_{xx} - \left[\frac{1}{6} Uh^2 + \frac{1}{3} U^3 \Delta t^2\right] f_{xxx}$	Unconditionally Stable
Lax-Friedrichs	$\frac{f_j^{n+1} - (f_{j+1}^n + f_{j-1}^n)/2}{\Delta t} + U \frac{(f_{j+1}^n - f_{j-1}^n)}{2h} = 0$	$\frac{Uh}{2}\left(\frac{1}{\lambda} - \lambda\right) f_{xx} + \frac{Uh^2}{3}(1 - \lambda^2) f_{xxx}$	Conditionally consistent Stable for $\lambda \le 1$

Computational Fluid Dynamics
Summary

$$f_t + U f_x = 0$$

Leap Frog	$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} + U \frac{f_{j+1}^n - f_{j-1}^n}{2h} = 0$	$\frac{Uh^2}{6}(\lambda^2 - 1) f_{xxx}$	Stable for $\lambda \le 1$
Lax-Wendroff I	$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{(f_{j+1}^n - f_{j-1}^n)}{2h} - U^2 \Delta t^2 \frac{(f_{j+1}^n - 2 f_j^n + f_{j-1}^n)}{2h^2} = 0$	$-\frac{Uh^2}{6}(1 - \lambda^2) f_{xxx} - \frac{Uh^3}{8} \lambda (1 - \lambda^2) f_{xxxx}$	Stable for $\lambda \le 1$
Lax-Wendroff II	$\frac{f_{j+1/2}^{n+1/2} - (f_{j+1}^n + f_j^n)/2}{\Delta t / 2} + U \frac{f_{j+1}^n - f_j^n}{h} = 0$ $\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{f_{j+1/2}^{n+1/2} - f_{j-1/2}^{n+1/2}}{h} = 0$	Same as LW-I	Stable for $\lambda \le 1$
MacCormack	$\frac{f_j^t - f_j^n}{\Delta t} + U \frac{(f_{j+1}^n - f_j^n)}{h} = 0$ $\frac{f_j^{n+1} - (f_j^n + f_j^t)/2}{\Delta t} + U \frac{(f_j^t - f_{j-1}^t)}{h} = 0$	Same as LW-I	Stable for $\lambda \le 1$

Computational Fluid Dynamics
Summary

$$f_t + U f_x = 0$$

Beam-Warming	$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{(3 f_j^n - 4 f_{j-1}^n + f_{j-2}^n)}{2h} - \frac{U^2 \Delta t}{2h^2}(f_j^n - 2 f_{j-1}^n + f_{j-2}^n) = 0$	$\frac{Uh^2}{6}(1-\lambda)(2-\lambda) f_{xxx} - \frac{Uh^3}{8}(1-\lambda)^2 (2-\lambda) f_{xxxx}$	Stable for $0 \le \lambda \le 2$
QUICK	$\frac{f_j^{n+1} - f_j^n}{\Delta t} + U \frac{(3 f_j^n + 6 f_{j-1}^n - f_{j-2}^n) - (3 f_{j+1}^n + 6 f_j^n - f_{j-1}^n)}{8h}$		Stable for $\lambda \le 1$

And Many More!

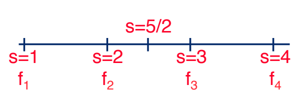
A large number of (conditionally) stable and accurate methods exists for hyperbolic equations with smooth solutions

Computational Fluid Dynamics

Higher order upwind QUICK

Computational Fluid Dynamics

QUICK (Quadratic Upstream Interpolation for Convective Kinematics)



Use to solve:

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

At s = 5/2

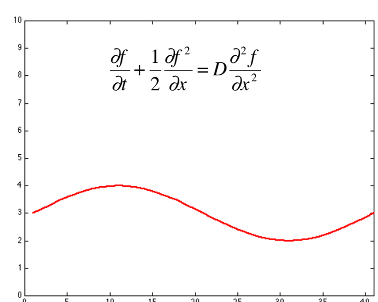
$$f_{5/2} = (1/8)[3 f_3 + 6 f_2 - f_1]$$

$$\left.\frac{\partial f^2}{\partial x}\right)_i \approx \frac{1}{h}\{f_{i+1/2}^2 - f_{i-1/2}^2\}$$

$$= \frac{1}{64h}\{[3 f_{i+1} + 6 f_i - f_{i-1}]^2 - [3 f_i + 6 f_{i-1} - f_{i-2}]^2\}$$

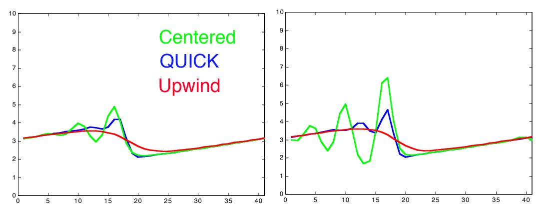
Computational Fluid Dynamics

Centered
QUICK
Upwind



Computational Fluid Dynamics

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



Re_cell=10 Re_cell=20

Computational Fluid Dynamics

Discontinuous solutions—shocks

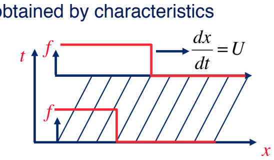
Computational Fluid Dynamics
Discontinuous Solutions

Consider the linear Advection Equation

$$\frac{\partial f}{\partial t}+U\frac{\partial f}{\partial x}=0 \qquad f(x,0)=\begin{cases} f_L & x<x_0 \\ f_R & x>x_0 \end{cases} \qquad (f_L>f_R)$$

The analytic solution is obtained by characteristics

$$\frac{dx}{dt}=U; \qquad \frac{df}{dt}=0;$$



Discontinuity of solution is allowed

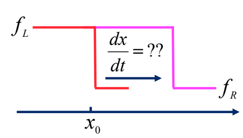
Computational Fluid Dynamics
Discontinuous Solutions

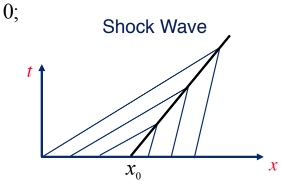
Inviscid Burgers' Equation

$$\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}=0 \qquad f(x,0)=\begin{cases} f_L & x<x_0 \\ f_R & x>x_0 \end{cases} \qquad (f_L>f_R)$$

Characteristics

$$\frac{dx}{dt}=f; \quad \frac{df}{dt}=0;$$

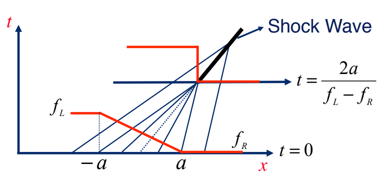




Computational Fluid Dynamics
Discontinuous Solutions

A slight variation of the initial condition – formation of shock

$$f(x,0)=\begin{cases} f_L & x<-a \\ \frac{1}{2}\left[(f_L+f_R)-(f_L-f_R)\frac{x}{a}\right] & -a<x<a \\ f_R & x>a \end{cases}$$

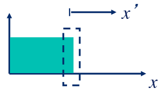


Computational Fluid Dynamics
Discontinuous Solutions

Shock Speed

Computational Fluid Dynamics
Discontinuous Solutions

The speed of the shock



Write: $x' = x - Ct$

$$\rightarrow \quad \frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x'}\frac{\partial x'}{\partial t}$$

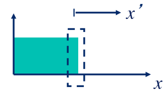
Substitute into: $\frac{\partial f}{\partial t} + \frac{\partial F}{\partial x} = 0$

$$\rightarrow \quad \frac{\partial f}{\partial t} - C\frac{\partial f}{\partial x'} + \frac{\partial F}{\partial x'} = 0 \quad \text{where} \quad \frac{\partial x'}{\partial t} = C$$

$$\rightarrow \quad \int_{\Delta\to 0}\left(\frac{\partial f}{\partial t} - C\frac{\partial f}{\partial x'} + \frac{\partial F}{\partial x'}\right)dx = 0$$

$$\int_{\Delta\to 0}\underbrace{\cancel{\left(\frac{\partial f}{\partial t}\right)}}_{0}dx - \int_{\Delta\to 0}\left(C\frac{\partial f}{\partial x'}\right)dx + \int_{\Delta\to 0}\left(\frac{\partial F}{\partial x'}\right)dx = 0$$

Computational Fluid Dynamics
Discontinuous Solutions



$$-\int_{\Delta\to 0}\left(C\frac{\partial f}{\partial x'}\right)dx + \int_{\Delta\to 0}\left(\frac{\partial F}{\partial x'}\right)dx = 0$$

$$\rightarrow \quad -C(f_R - f_L) + (F_R - F_L) = 0$$

Rankine-Hugoniot relations

$$\rightarrow \quad C = \frac{F_R - F_L}{f_R - f_L}$$

Computational Fluid Dynamics
Discontinuous Solutions

Example

$$\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x} = 0 \qquad F = \frac{1}{2}f^2$$

$$C = \frac{F_R - F_L}{f_R - f_L} = \frac{1}{2}\frac{f_R^2 - f_L^2}{f_R - f_L} = \frac{1}{2}\frac{\cancel{(f_R - f_L)}(f_R + f_L)}{\cancel{f_R - f_L}}$$

$$\rightarrow \quad C = \frac{1}{2}(f_R + f_L)$$

Computational Fluid Dynamics

The Entropy Conditions

Computational Fluid Dynamics
The Entropy Conditions

Inviscid Burgers' Equation

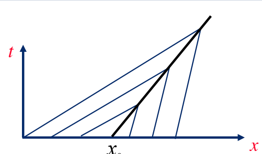
$$\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x} = 0$$

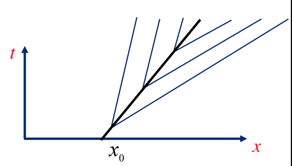
The transformation

$$x \to -x; \quad t \to -t$$

Leaves the equation unchanged but results in an unphysical solution.

The entropy condition is used to select the correct solution





Computational Fluid Dynamics
The Entropy Conditions

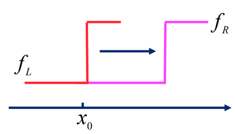
Reverse Shock (?)

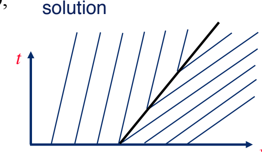
$$\frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x} = 0 \qquad f(x,0) = \begin{cases} f_L & x < x_0 \\ f_R & x > x_0 \end{cases} \qquad (f_L < f_R)$$

Characteristics

$$\frac{dx}{dt} = f; \quad \frac{df}{dt} = 0;$$

Unstable, entropy-violating solution





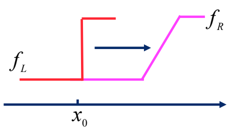
Computational Fluid Dynamics
The Entropy Conditions

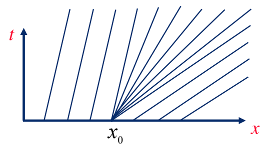
Rarefaction Wave (physically correct solution)

$$\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}=0 \qquad f(x,0)=\begin{cases} f_L & x<x_0 \\ f_R & x>x_0 \end{cases} \qquad (f_L<f_R)$$

Characteristics

$$\frac{dx}{dt}=f;\quad \frac{df}{dt}=0;$$





Computational Fluid Dynamics
The Entropy Conditions

Weak solutions to hyperbolic equations may not be unique.

How can we find a physical solution out of many weak solutions?

In fluid mechanics, the actual physics always includes dissipation, i.e. in the form of viscous Burgers' equation:

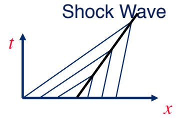
$$\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}=\varepsilon\frac{\partial^2 f}{\partial x^2}$$

Therefore, what we are truly seeking is the solution to the viscous Burgers' equation in the limit of $\varepsilon \to 0$

Computational Fluid Dynamics
Entropy Condition

For a conservation equation

$$\frac{\partial f}{\partial t}+\frac{\partial F(f)}{\partial x}=0$$



Entropy Condition:
A discontinuity propagating with speed C satisfies the entropy condition if

Version I: $F'(f_L)>C>F'(f_R)$

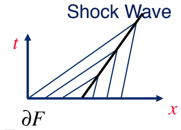
Version II: $\dfrac{F(f)-F(f_L)}{f-f_L}\geq C\geq\dfrac{F(f)-F(f_R)}{f-f_R}$ for $f_L\geq f\geq f_R$

And some others…

Computational Fluid Dynamics
Entropy Condition

Given a conservation equation

$$\frac{\partial f}{\partial t}+\frac{\partial F(f)}{\partial x}=0$$



Rewrite in "characteristic" form

$$\frac{\partial f}{\partial t}+\frac{\partial F}{\partial f}\frac{\partial f}{\partial x}=0 \quad \text{where:} \quad \frac{dt}{ds}=1;\quad \frac{dx}{ds}=\frac{\partial F}{\partial f}$$

or: $\dfrac{dx}{dt}=\dfrac{\partial F}{\partial f}=F'(f)$

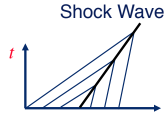
The Entropy Condition states that the characteristics must "enter" the discontinuity. Thus, its speed C satisfies must satisfy

$$F'(f_L)>C>F'(f_R)$$

Computational Fluid Dynamics
Entropy Condition

Similarly, the shock speed is given by

$$C=\frac{F_R-F_L}{f_R-f_L}$$



Thus

$$\frac{F(f)-F(f_L)}{f-f_L}\geq C\geq\frac{F(f)-F(f_R)}{f-f_R} \qquad \text{for } f_L\geq f\geq f_R$$

Means that the hypothetical shock speed for values of f between the left and the right state must give shock speeds that are larger on the left and smaller on the right.

Computational Fluid Dynamics

Conservative discretization

Computational Fluid Dynamics
Conservative Schemes

In finite volume method, equations in conservative forms are needed in order to satisfy conservation properties.

As an example, consider a 1-D equation

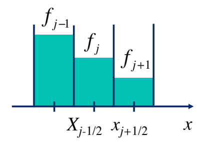
$$\frac{\partial f(x,t)}{\partial t}+\frac{\partial F[f(x,t)]}{\partial x}=0$$

where F denotes a general advection/diffusion term, e.g.

$$F=\frac{1}{2}f^2;\quad F=\mu(x)\frac{\partial f}{\partial x}$$

Computational Fluid Dynamics
Conservative Schemes

Integrating over the domain L,



$$\int_L \frac{\partial f}{\partial t}dx+\int_L \frac{\partial F}{\partial x}dx=0$$

$$F(L)-F(0)=0\quad \Rightarrow \frac{d}{dt}\int_L f dx=0$$

If $F=0$ at the end points of the domain, f is conserved.

In discretized form:

$$\int_L \frac{\partial F}{\partial x}dx=\sum \frac{F_{j+1/2}-F_{j-1/2}}{\cancel{\Delta x}}\cancel{\Delta x}$$

$$=\left[\cdots+\cancel{F_{j-1/2}}-F_{j-3/2}+\cancel{F_{j+1/2}}-\cancel{F_{j-1/2}}+F_{j+3/2}-\cancel{F_{j+1/2}}+\cdots\right]$$

$$=F_L-F_0$$

Computational Fluid Dynamics
Conservative Schemes

Examples of Conservative Form

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x}\left(\frac{1}{2}f^2\right)=0 \quad \text{versus} \quad \frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}=0$$

Discretize using upwind

$$\frac{\partial}{\partial x}\left(\frac{1}{2}f^2\right)\approx\frac{1}{2h}\left(f_i^2-f_{i-1}^2\right)$$ Conservative

$$f\frac{\partial f}{\partial x}\approx\frac{f_i}{h}\left(f_i-f_{i-1}\right)$$ Non-conservative

Computational Fluid Dynamics
Conservative Schemes

$$\left.\frac{\partial}{\partial x}\left(\frac{1}{2}f^2\right)\right)_i\approx\frac{1}{2h}\left(f_i^2-f_{i-1}^2\right)$$

$$\int_L \frac{\partial F}{\partial x}dx\approx\sum F_{j+1/2}-F_{j-1/2}=$$

$$\cdots+\cancel{f_{i-1}^2}-f_{i-2}^2+\cancel{f_i^2}-\cancel{f_{i-1}^2}+f_{i+1}^2-\cancel{f_i^2}+\cdots$$

$$\left.f\frac{\partial f}{\partial x}\right)_i\approx\frac{f_i}{h}\left(f_i-f_{i-1}\right)$$

$$\int_L \frac{\partial F}{\partial x}dx\approx\sum F_{j+1/2}-F_{j-1/2}=$$

$$\cdots+f_{i-1}^2-f_{i-1}f_i+f_i^2-f_if_{i-1}+f_{i+1}^2-f_{i+1}f_i+\cdots$$

Computational Fluid Dynamics
Conservative Schemes

Another example (variable diffusion coefficient)

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x}\left(\mu(x)\frac{\partial f}{\partial x}\right)=0$$

Discretize $\frac{\partial}{\partial x}\left(\mu(x)\frac{\partial f}{\partial x}\right)$ versus $\mu\frac{\partial^2 f}{\partial x^2}+\frac{\partial\mu}{\partial x}\frac{\partial f}{\partial x}$

Conservative — Non-conservative

Computational Fluid Dynamics
Conservative Schemes

Conservation of higher order quantities

Consider:

$$\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}=0\qquad f(\infty)=f(-\infty)=0$$

$$f\left(\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}\right)=0$$

$$\frac{\partial}{\partial t}\frac{f^2}{2}+\frac{\partial}{\partial x}\frac{f^3}{3}=0$$

Similarly, it can be shown that

$$\frac{d}{dt}\int\frac{f^n}{n}dx=0$$

Integrate:

$$\frac{d}{dt}\int\frac{f^2}{2}dx=-\int\frac{\partial}{\partial x}\frac{f^3}{3}dx=\left[\frac{f^3}{3}\right]_{-\infty}^{\infty}=0$$

Computational Fluid Dynamics

Generally it is believed that conservative schemes are superior to non-conservative ones and that the more conserved quantities the discrete approximation preserves, the better the scheme. While mostly true, there are exceptions as we will discuss later!

Computational Fluid Dynamics
Discontinuous Solutions

Conservative Schemes are guarantied to give the correct Shock Speed since they correspond to a direct application of the conservation principles.

Non-conservative schemes may or may not do so.

Computational Fluid Dynamics
Conservative Method

Conservation and shock speed

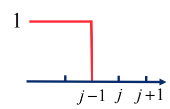
Example: inviscid Burgers equation:

$$\frac{\partial f}{\partial t}+f\frac{\partial f}{\partial x}=0 \quad \text{or} \quad \frac{\partial f}{\partial t}+\frac{\partial}{\partial x}\left(\frac{1}{2}f^2\right)=0$$

In capturing the correct solution behavior for discontinuous Initial data, conservative methods are essential (Lax).

Computational Fluid Dynamics
Conservative Method

Example: for inviscid Burgers equation with discontinuous initial data



Consider upwind and forward Euler scheme:

Non-conservative form $f_t + ff_x = 0$

$$f_j^{n+1}=f_j^n-\frac{\Delta t}{h}f_j^n\left(f_j^n-f_{j-1}^n\right)=0 \quad \text{Never moves!}$$

Conservative form $f_t+\left(\frac{1}{2}f^2\right)_x=0$

$$f_j^{n+1}=f_j^n-\frac{\Delta t}{2h}\left((f_j^n)^2-(f_{j-1}^n)^2\right)=\frac{\Delta t}{2h}$$

Computational Fluid Dynamics

Advecting a shock with several schemes

Computational Fluid Dynamics

Example Problem: Linear Wave Equation

$$\frac{\partial f}{\partial t}+U\frac{\partial f}{\partial x}=0, \quad -\infty<x<\infty,\ t\geq 0$$

$$f(x,0)=\begin{cases}1 & x<0\\ 0 & x>0\end{cases}$$

Exact Solution: $f(x-Ut)$

Apply various numerical methods

Computational Fluid Dynamics

$$f_j^{n+1} = f_j^n - \frac{\Delta t}{h} U (f_j^n - f_{j-1}^n)$$ Upwind

$$f_j^{n+1} = f_j^{n-1} - \frac{U \Delta t}{h} \left(f_{j+1}^n - f_{j-1}^n \right)$$ Leap-frog

Lax-Wendroff

$$f_j^{n+1} = f_j^n - \frac{U \Delta t}{2h} \left(f_{j+1}^n - f_{j-1}^n \right) + \frac{U^2 \Delta t^2}{2h^2} \left(f_{j+1}^n - 2 f_j^n + f_{j-1}^n \right)$$

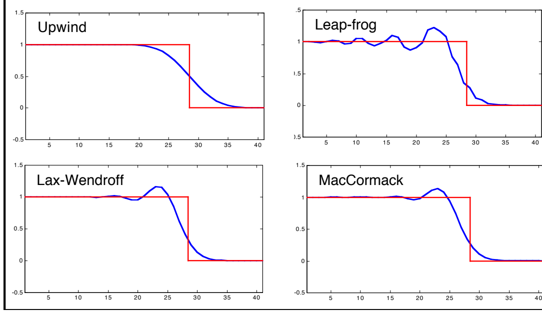
$$f_j^t = f_j^n - U \frac{\Delta t}{h} \left(f_{j+1}^n - f_j^n \right)$$

MacCormack

$$f_j^{n+1} = \frac{1}{2} \left[f_j^n + f_j^t - U \frac{\Delta t}{h} \left(f_j^t - f_{j-1}^t \right) \right]$$

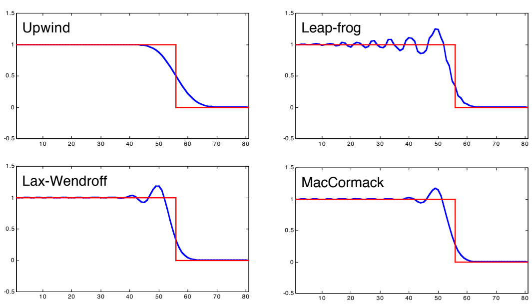
Computational Fluid Dynamics

Comparison: h=0.1; dt= 0.05;n=41, time=2.75



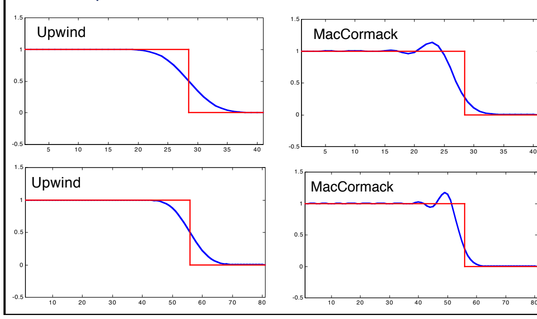
Computational Fluid Dynamics

Comparison: h=0.05; dt= 0.025;n=81, time=2.75



Computational Fluid Dynamics

Comparison: n=41 and n=81, time=2.75



Computational Fluid Dynamics

Observation 1:
Second-order methods tends to capture shaper solution (better accuracy), but they produce wiggly solutions.

Observation 2:
First-order methods are dissipative and less accurate, but the solution does not oscillate.
(preserves monotonicity).

Computational Fluid Dynamics
http://www.nd.edu/~gtryggva/CFD-Course/

Classical Methods

Discontinuous solutions

Entropy conditions

Shock speed

Conservative discretization