High-Fidelity Simulations for Turbulent Flows

Luca Sciacovelli

DynFluid Laboratory
Arts et Métiers Institute of Technology
http://savoir.ensam.eu/moodle

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Part V

Discretization of the Navier-Stokes equations

1st order PDE - Characteristics (I)

- PDE order determined by **highest derivatives**
  - **Linear**: no powers or products of the unknown functions or its partial derivatives are present

$$x\frac{\partial w}{\partial x} + y\frac{\partial w}{\partial y} = w, \qquad \frac{\partial w}{\partial x} + \frac{\partial w}{\partial y} + 2xw = 0$$

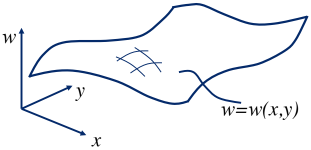
  - **Quasi-linear** if it is true for the partial derivatives of the highest order

$$w\frac{\partial^2 w}{\partial x^2} + \left(\frac{\partial w}{\partial y}\right)^2 = w, \qquad x^2\frac{\partial w}{\partial x} + y^2\frac{\partial w}{\partial y} = w^2$$

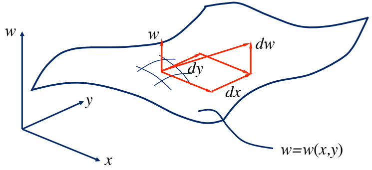
- Consider the 1st-order linear PDE

$$\boxed{a\frac{\partial w}{\partial x} + b\frac{\partial w}{\partial y} = c}$$

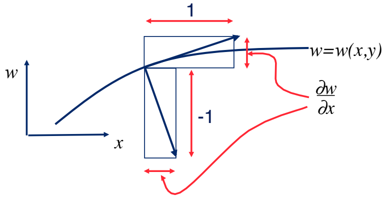
with $a = a(x, y, w), b = b(x, y, w), c = c(x, y, w)$



- Arbitrary change in w: $\mathrm{d}w = \dfrac{\partial w}{\partial x}\mathrm{d}x + \dfrac{\partial w}{\partial y}\mathrm{d}y$



- Normal vector to the curve $w = w(x, y)$



- Same argument in y-direction, thus

$$\vec{n} = \left(\frac{\partial w}{\partial x}, \frac{\partial w}{\partial y}, -1\right)$$

1st order PDE - Characteristics (II)

The original equation and the condition for a small change can be rewritten as

$$a\frac{\partial w}{\partial x} + b\frac{\partial w}{\partial y} = c \implies \left(\frac{\partial w}{\partial x}, \frac{\partial w}{\partial y}, -1\right) \cdot (a, b, c) = 0$$

$$\mathrm{d}w = \frac{\partial w}{\partial x}\mathrm{d}x + \frac{\partial w}{\partial y}\mathrm{d}y \implies \left(\frac{\partial w}{\partial x}, \frac{\partial w}{\partial y}, -1\right) \cdot (\mathrm{d}x, \mathrm{d}y, \mathrm{d}w) = 0$$

- Both (a, b, c) and $(\mathrm{d}x, \mathrm{d}y, \mathrm{d}w)$ are normal to the surface
- Picking the displacement in the direction of (a, b, c):

$$(\mathrm{d}x, \mathrm{d}y, \mathrm{d}w) = \mathrm{d}s(a, b, c)$$

And separating the components:

$$\underbrace{\frac{\mathrm{d}x}{\mathrm{d}s} = a, \quad \frac{\mathrm{d}y}{\mathrm{d}s} = b,}_{\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{a}{b}} \quad \frac{\mathrm{d}w}{\mathrm{d}s} = c,$$

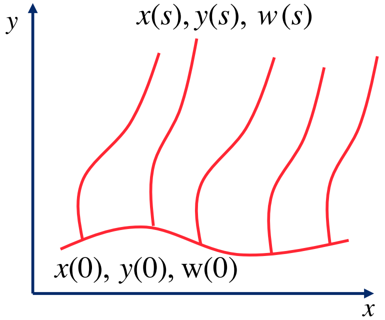
- The 3 equations specify lines in the $x - y$ plane

Characteristics

Given the initial conditions:

$$x = x(s, t_0), \quad y = y(s, t_0), \quad w = w(s, t_0)$$

The equations can be integrated in time:

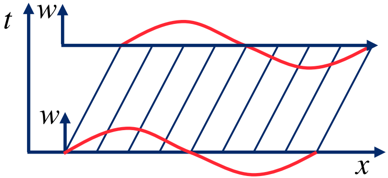


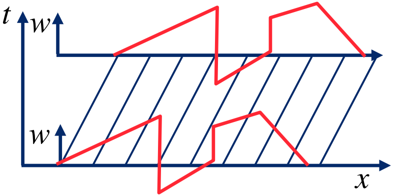
Linear advection equation

$$\boxed{\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = 0} \implies \text{Characteristics: } \frac{dt}{ds} = 1, \quad \frac{dx}{ds} = a, \quad \frac{dw}{ds} = 0 \quad \text{or} \quad \frac{dx}{dt} = a, \quad dw = 0$$

The solution moves along straight characteristics without changing its value!

Graphically: $w(x,t) = w_{t=0}(x - at)$





- Solution: $w(x,t) = f(x - at)$ with $f(x) = w(x, t = 0)$
- Verified by direct substitution: set $\eta(x,t) = x - at$, then:

$$\frac{\partial w}{\partial t} = \frac{\partial f}{\partial \eta}\frac{\partial \eta}{\partial t} = \frac{\partial f}{\partial \eta}(-a)$$
$$\frac{\partial w}{\partial x} = \frac{\partial f}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{\partial f}{\partial \eta}(1)$$

- Replace into the original equation:

$$\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = \cancel{\partial f/\partial\eta(-a)} + \cancel{a\frac{\partial g}{\partial \eta}} = 0$$

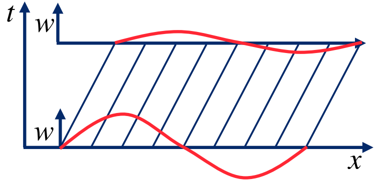
- Since the solution propagates along characteristics independently of the solution at the next spatial point, there is no requirement that it is differentiable or even continuous

Linear advection equation

- **Linear advection with source term**: $$\boxed{\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = -w}$$

$$\textbf{Characteristics}: \quad \frac{dt}{ds} = 1, \quad \frac{dx}{ds} = a, \quad \frac{dw}{ds} = -w$$

$$\text{or} \quad \frac{dx}{dt} = a, \quad \frac{dw}{dt} = -w \quad \Longrightarrow \quad w = w(0)e^{-t}$$



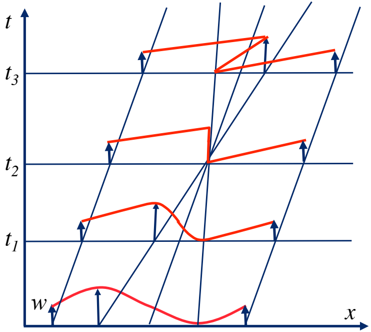
Moving wave with decaying amplitude

- **Quasi-linear advection equation**: $$\boxed{\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial x} = 0}$$

$$\textbf{Characteristics}: \quad \frac{dt}{ds} = 1, \quad \frac{dx}{ds} = w, \quad \frac{dw}{ds} = 0$$

$$\text{or} \quad \frac{dx}{dt} = w, \quad dw = 0$$

- The slope of the characteristics depends on the value of $w(x, t)$
- Why unphysical solutions? Because mathematical equation neglects some physical process (dissipation)
- Additional (entropy) condition required to pick out the physically relevant solution, using conservation of w



Multi-valued solution..

2nd order PDE - Characteristics (I)

$$\boxed{a\frac{\partial^2 w}{\partial x^2} + b\frac{\partial^2 w}{\partial x \partial y} + c\frac{\partial^2 w}{\partial y^2} = d} \qquad (\star)$$

with

$$\begin{aligned} a &= a(x, y, w, w_x, w_y) \\ b &= b(x, y, w, w_x, w_y) \\ c &= c(x, y, w, w_x, w_y) \\ d &= d(x, y, w, w_x, w_y) \end{aligned}$$

- First write the PDE as a system of 1st-order eqs:
  - Define $f = \dfrac{\partial w}{\partial x}$ and $g = \dfrac{\partial w}{\partial y}$
  - Then $(\star)$ becomes: $a\dfrac{\partial f}{\partial x} + b\dfrac{\partial f}{\partial y} + c\dfrac{\partial g}{\partial y} = d$
  - The 2nd eq. is obtained from:

$$\frac{\partial^2 w}{\partial x \partial y} = \frac{\partial^2 w}{\partial y \partial x} \implies \frac{\partial g}{\partial x} - \frac{\partial f}{\partial y} = 0$$

- $(\star)$ is then equivalent to

$$\begin{cases} a\dfrac{\partial f}{\partial x} + b\dfrac{\partial f}{\partial y} + c\dfrac{\partial g}{\partial y} = d \\ \dfrac{\partial g}{\partial x} - \dfrac{\partial f}{\partial y} = 0 \end{cases}$$

  - Any high-order PDE can be rewritten as a system of 1st-order equations
  - In matrix form, one has

$$\begin{bmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial g}{\partial x} \end{bmatrix} + \underbrace{\begin{bmatrix} \dfrac{b}{a} & \dfrac{c}{a} \\ -1 & 0 \end{bmatrix}}_{A} \cdot \begin{bmatrix} \dfrac{\partial f}{\partial y} \\ \dfrac{\partial g}{\partial y} \end{bmatrix} = \begin{bmatrix} \dfrac{d}{a} \\ 0 \end{bmatrix}$$

$$\text{or} \quad \vec{u}_x + A\vec{u}_y = \vec{s} \quad \text{with} \quad \vec{u} = \begin{bmatrix} f \\ g \end{bmatrix}$$

  - Are there lines in the $x - y$ plane, along which the solution is determined by an ODE?

2nd order PDE - Characteristics (II)

The **total derivative** is:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial f}{\partial x} + \alpha\frac{\partial f}{\partial y} \quad \text{with} \quad \alpha = \frac{\partial y}{\partial x}$$

- Rate of change of f with x, along the line $y = y(x)$
- If there are lines (determined by α) where the solution is governed by ODE's, then it must be possible to rewrite the eqs. such that the result contains only α and the total derivatives!
  - Add the original equations:

$$\lambda_1\left(\frac{\partial f}{\partial x} + \frac{b}{a}\frac{\partial f}{\partial y} + \frac{c}{a}\frac{\partial g}{\partial y}\right) + \lambda_2\left(\frac{\partial g}{\partial x} - \frac{\partial f}{\partial y}\right) = \lambda_1\frac{d}{a}$$

  - And compare to

$$\lambda_1\left(\frac{\partial f}{\partial x} + \alpha\frac{\partial f}{\partial y}\right) + \lambda_2\left(\frac{\partial g}{\partial x} + \alpha\frac{\partial g}{\partial y}\right) = \lambda_1\frac{d}{a}$$

  for some λ's and α

- The two systems are equal if:

$$(\star)\begin{cases}\lambda_1\frac{b}{a} - \lambda_2 = \lambda_1\alpha \\ \lambda_1\frac{c}{a} = \lambda_2\alpha\end{cases} \Longrightarrow \begin{bmatrix}\frac{b}{a} - \alpha & -1 \\ \frac{c}{a} & -\alpha\end{bmatrix}\cdot\begin{bmatrix}\lambda_1 \\ \lambda_2\end{bmatrix} = \begin{bmatrix}0 \\ 0\end{bmatrix}$$

- Characteristic lines exist if $(\star)$ is verified
- The system can be recast as

$$\underbrace{\begin{bmatrix}\frac{b}{a} & -1 \\ \frac{c}{a} & 0\end{bmatrix}}_{A^T}\cdot\begin{bmatrix}\lambda_1 \\ \lambda_2\end{bmatrix} - \begin{bmatrix}-\alpha & 0 \\ 0 & -\alpha\end{bmatrix}\cdot\begin{bmatrix}\lambda_1 \\ \lambda_2\end{bmatrix} = \begin{bmatrix}0 \\ 0\end{bmatrix}$$

$$\Longrightarrow (A^T - \alpha I)\vec{\lambda} = 0$$

  - It has a solution $\iff$ the determinant is zero!

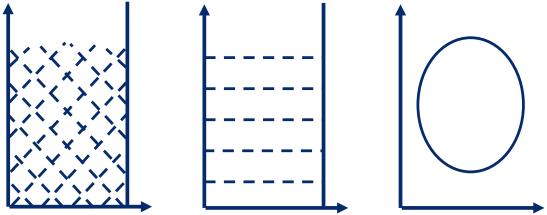
$$-\alpha\left(\frac{b}{a} - \alpha\right) + \frac{c}{a} = 0 \iff \boxed{\alpha = \frac{1}{2a}\left(b \pm \sqrt{b^2 - 4ac}\right)}$$

1. $b^2 - 4ac > 0$: **2 real characteristics: hyperbolic**
2. $b^2 - 4ac = 0$: **1 real characteristic: parabolic**
3. $b^2 - 4ac < 0$: **0 real characteristics: elliptic**

Examples

Comparing with the standard form $\boxed{a\frac{\partial^2 w}{\partial x^2} + b\frac{\partial^2 w}{\partial x \partial y} + c\frac{\partial^2 w}{\partial y^2} = d}$

	Equation	a	b	c	d	$b^2 - 4ac$	Type
Wave propagation	$\frac{\partial^2 w}{\partial x^2} - c^2\frac{\partial^2 w}{\partial y^2} = 0$	1	0	$-c^2$	0	$4c^2 > 0$	**Hyperbolic**
Diffusion equation	$\frac{\partial w}{\partial x} - \nu\frac{\partial^2 w}{\partial y^2} = 0$	0	0	$-\nu$	0	0	**Parabolic**
Laplace equation	$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} = 0$	1	0	1	0	$-4 < 0$	**Elliptic**



Hyperbolic **Parabolic** **Elliptic**

- Why the classification is so important?
  - Different initial and boundary conditions
  - Different physics
  - Different numerical methods

Examples

Incompressible Navier–Stokes

$$\underbrace{\frac{\partial u}{\partial t}}_{(1)} + \underbrace{u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{1}{\rho}\frac{\partial p}{\partial x}}_{(2)} + \underbrace{\nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)}_{(3)}$$

	Steady		Unsteady	
		Type		**Type**
Viscous flow	(3)	Elliptic	(1)+(3)	Parabolic
Inviscid flow	(2)	$Ma \ll 1$: Elliptic $Ma > 1$: Hyperbolic	(1)+(2)	Hyperbolic
Thin shear layers	(2)+(3)	Parabolic	(1)+(3)	Parabolic

- NS eqs. contains three equation types having their own characteristic behavior
- Depending on the configuration, one behavior can be dominant. Examples:
  - **Inviscid flows**:
    - $Ma \ll 1$: pressure disturbances travel faster than flow speed $\Longrightarrow$ **elliptic** character
    - $Ma > 1$: pressure disturbances cannot travel upstream $\Longrightarrow$ **hyperbolic** character
  - **Thin shear layers**: $\dfrac{\partial(\bullet)}{\partial x} \ll \dfrac{\partial(\bullet)}{\partial y}$ $\Longrightarrow$ only one second order term $\Longrightarrow$ **parabolic** character

Ill-posed problems

Consider the IVP: $\boxed{\dfrac{\partial^2 w}{\partial t^2} = -\dfrac{\partial^2 w}{\partial x^2}}$ with w^0 and $\dfrac{\partial w^0}{\partial t}$ given on the boundaries

- This is simply **Laplace's equation**, which has a solution if $w(t)$ or $\dfrac{\partial w}{\partial t}$ are given on the boundaries
- Here, it appears as an IVP (BCs given only at $t = 0$)

- **General solution**: $w(x,t) = \sum_k \widehat{w}_k(t) e^{ikx}$

  $\widehat{w}_k(t)$ depending on ICs
- Replacing in the equation: $\dfrac{d^2 \widehat{w}_k}{dt^2} = k^2 \widehat{w}_k$

  For which one has $\widehat{w}_k(t) = Ae^{kt} + Be^{-kt}$
  - A, B determined by the ICs $\widehat{w}_k^0$ and $ik\widehat{w}_k^0$
  - $\widehat{w}_k \to \infty$ as $t \to \infty$: **Ill-posed problem!**
- Similar behavior obtained for diffusion equation with $\nu < 0$: unbounded growth rate for high-wavenumber modes

- Ill-posed problems generally appear when ICs or BCs and the equation type do not match, or because small but important higher-order effects have been neglected
- They result in exponential growth of small perturbations, so that the solution does not depend continuously on the initial data
- Examples: inviscid vortex sheet roll-up, multiphase flow models, viscoelastic constitutive models, ..

Remainder: the NS equations

$$\frac{\partial w}{\partial t} + \nabla \cdot (\mathbf{F}^e - \mathbf{F}^v) = 0 \qquad w = \begin{bmatrix} \rho \\ \rho\vec{u} \\ \rho E \end{bmatrix} \qquad F^e = \begin{bmatrix} \rho\vec{u} \\ \rho\vec{u}\vec{u} + p\mathbf{I} \\ \rho\vec{u}H \end{bmatrix} \qquad F^v = \begin{bmatrix} 0 \\ \vec{\vec{\tau}} \\ \vec{\vec{\tau}}\vec{u} - \vec{q} \end{bmatrix}$$

- **Boundary conditions**
  - **Inlet/Outlet**: viscous effects negligible (no BLs): **same BCs** as in inviscid flows hold
  - **Walls**: no-slip condition ($\vec{u} = \vec{u}_{\text{wall}}$) + condition on T (Adiabatic, $\vec{q} = 0$, or Isothermal, $T = T_{\text{wall}}$)
- For aerodynamic problems, $Pr \approx 0.72$ and $Re \gg 1$
  - Most of the flow dominated by inviscid effects
  - Viscous effects important in regions with strong gradients
  - Shock waves too thin to be resolved in common use meshes $\Longrightarrow$ **captured** or seen as **discontinuities**
- A good NS solver should be, first of all, a good **Euler solver**
  - Already seen in the Basics of Numerical Methods course
  - We focus on the discretisation of viscous terms and interactions with convective terms and time derivatives (stability issues)

Model problem: stability analysis

Consider the wave equation:

$$\boxed{\frac{\partial^2 w}{\partial t^2} - c^2\frac{\partial^2 w}{\partial x^2} = 0} \quad \text{write as} \quad \begin{cases} \dfrac{\partial f}{\partial t} - c^2\dfrac{\partial g}{\partial x} = 0 \\ \dfrac{\partial g}{\partial t} - \dfrac{\partial f}{\partial x} = 0 \end{cases} \quad \text{or} \quad \begin{bmatrix} \dfrac{\partial f}{\partial t} \\ \dfrac{\partial g}{\partial t} \end{bmatrix} + \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \cdot \begin{bmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial g}{\partial x} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Most of the issues involved can be addressed by examining the linear advection equation $\boxed{\dfrac{\partial w}{\partial t} + a\dfrac{\partial w}{\partial x} = 0}$

Example: **Upwind method for advection equation** ($\mathcal{O}(\Delta t, \Delta x)$ accurate)

- Write the solution as $\widehat{w}_j^n = \widehat{w}^n e^{ikx_j}$
- Replace in the discretized equation

$$\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = 0$$

$$\frac{w_j^{n+1} - w_j^n}{\Delta t} + a\frac{w_j^n - w_{j-1}^n}{\Delta x} = 0$$

$$\frac{\widehat{w}_j^{n+1} - \widehat{w}_j^n}{\Delta t} + a\frac{\widehat{w}_j^n - \widehat{w}_{j-1}^n}{\Delta x} = 0$$

$$\frac{\widehat{w}^{n+1} - \widehat{w}^n}{\Delta t} + \frac{a\widehat{w}^n}{\Delta x}\left(1 - e^{-ik\Delta x}\right) = 0$$

- Evaluate the **amplification factor** G:

$$\Longrightarrow \quad G = \frac{\widehat{w}^{n+1}}{\widehat{w}^n} = 1 - \frac{a\Delta t}{\Delta x}\left(1 - e^{-ik\Delta x}\right)$$
$$= 1 - \dot{a}\left(1 - e^{-ik\Delta x}\right) \quad \text{with} \quad \dot{a} = \frac{a\Delta t}{\Delta x}$$
$$= 1 - \dot{a} + \dot{a}e^{-ik\Delta x} = 1 - \dot{a} + \dot{a}e^{-i\beta}$$

- **Stability** $\Longleftrightarrow$ errors remain **bounded** (*i.e.* $|G| < 1$)
- Need to find values of $\dot{a}$ for which $|G| < 1$!

Two classical methods: 1) **Analytical**, 2) **Graphical**

Von Neumann Stability Analysis

$$G = 1 - \dot{a} + \dot{a}e^{-i\beta} = (1 - \dot{a} + \dot{a}\cos\beta) - i(\dot{a}\sin\beta) \qquad (\star)$$

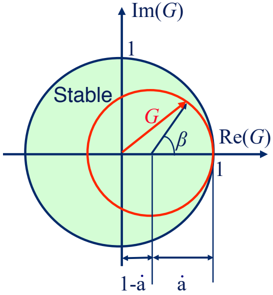
Analytical method

$$\begin{aligned}
|G|^2 &= (1 - \dot{a} + \dot{a}\cos\beta)^2 + (\dot{a}\sin\beta)^2 \\
&= (1-\dot{a})^2 + 2(1-\dot{a})\dot{a}\cos\beta + \dot{a}^2\cos^2\beta + \dot{a}^2\sin^2\beta \\
&= (1-\dot{a})^2 + 2(1-\dot{a})\dot{a}\cos\beta + \dot{a}^2 \\
&= 1 - 2\dot{a} + 2\dot{a}^2 + 2(1-\dot{a})\dot{a}\cos\beta \\
&= 1 + 2\dot{a}(1-\dot{a})(1-\cos\beta) \leq 1 \\
&\iff \dot{a}(1-\dot{a})(\cos\beta - 1) \leq 0
\end{aligned}$$

- Since $\cos\beta - 1 \leq 0 \quad \forall\beta$, then

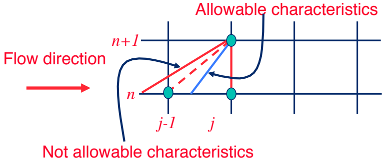
$$|G|^2 \leq 1 \iff \dot{a}(1-\dot{a}) \geq 0$$
$$\iff \boxed{0 \leq \dot{a} \leq 1}$$

Graphical method



- Green region: stability zone ($|G| < 1$)
- Red circle: representation of ($\star$)
- Circle must be contained in green region, thus:
- $\boxed{|G|^2 \leq 1 \iff \dot{a} \leq 1}$

The signal must travel less than 1 Δx in 1 Δt!



Generalized Upwind Scheme

$$w_j^{n+1} = \begin{cases} w_j^n - \dfrac{a\Delta t}{\Delta x}(w_j^n - w_{j-1}^n) & a > 0 \\ w_j^n - \dfrac{a\Delta t}{\Delta x}(w_{j+1}^n - w_j^n) & a < 0 \end{cases}$$

Generalized case: define

$$a^+ = \frac{1}{2}(a + |a|) \qquad a^- = \frac{1}{2}(a - |a|)$$

And combine into a single expression:

$$w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x}\left[a^+(w_j^n - w_{j-1}^n) + a^-(w_{j+1}^n - w_j^n)\right]$$

Replacing a^+ and a^- with their definitions:

$$w_j^{n+1} = w_j^n - \frac{a\Delta t}{2\Delta x}(w_{j+1}^n - w_{j-1}^n) + \frac{|a|\Delta t}{2\Delta x}(w_{j+1}^n - 2w_j^n + w_{j-1}^n)$$

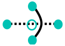
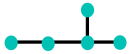
- Central difference + numerical viscosity obtained! $\nu_{\text{num}} = \dfrac{|a|\Delta x}{2}$

Summary: First-order schemes

$$\boxed{\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = 0} \qquad \dot{a} = \frac{a\Delta t}{\Delta x}$$

Name / Stencil	Scheme	Error term	Stability
FTCS 	$\frac{w_j^{n+1} - w_j^n}{\Delta t} + a\frac{w_{j+1}^n - w_{j-1}^n}{2\Delta x} = 0$	$-\Delta t\frac{a^2}{2}w_{xx} - \frac{a\Delta x^2}{6}(1+2\dot{a}^2)w_{xxx}$	Unconditionally Unstable
Upwind 	$\frac{w_j^{n+1} - w_j^n}{\Delta t} + a\frac{w_j^n - w_{j-1}^n}{\Delta x} = 0$	$\frac{a\Delta x}{2}(1-\dot{a})w_{xx} - \frac{a\Delta x^2}{6}(2\dot{a}^2 - 3\dot{a} + 1)w_{xxx}$	Stable for $\dot{a} \leq 1$
Implicit 	$\frac{w_j^{n+1} - w_j^n}{\Delta t} + a\frac{w_{j+1}^{n+1} - w_{j-1}^{n+1}}{2\Delta x} = 0$	$\frac{a^2\Delta t}{2}w_{xx} - \left[\frac{1}{6}a\Delta x^2 + \frac{1}{3}a^3\Delta t^2\right]w_{xxx}$	Unconditionally Stable
Lax-Friedrichs 	$\frac{w_j^{n+1} - \frac{1}{2}(w_{j+1}^n + w_{j-1}^n)}{\Delta t} + a\frac{w_{j+1}^n - w_{j-1}^n}{2\Delta x} = 0$	$\frac{a\Delta x}{2}\left[\frac{1}{\dot{a}} - \dot{a}\right]w_{xx} + \frac{a\Delta x^2}{3}(1-\dot{a}^2)w_{xxx}$	Stable for $\dot{a} \leq 1$

Summary: Second-order schemes

Name / Stencil	Scheme	Error term	Stability
Leap Frog 	$\frac{w_j^{n+1}-w_j^{n-1}}{2\Delta t}+a\frac{w_{j+1}^n-w_{j-1}^n}{2\Delta x}=0$	$\frac{a\Delta x^2}{6}(\dot{a}^2-1)w_{xxx}$	Stable for $\dot{a}\leq 1$
Lax-Wendroff I 	$\frac{w_j^{n+1}-w_j^n}{\Delta t}+a\frac{w_{j+1}^n-w_{j-1}^n}{2\Delta x}$ $-a^2\Delta t^2\frac{w_{j+1}^n-2w_j^n+w_{j-1}^n}{2\Delta x^2}=0$	$-\frac{a\Delta x^2}{6}(1-\dot{a}^2)w_{xxx}$ $-\frac{a\Delta x^3}{8}\dot{a}(1-\dot{a}^2)w_{xxxx}$	Stable for $\dot{a}\leq 1$
Lax-Wendroff II  (Lax + Leapfrog)	$\frac{w_{j+1/2}^{n+1/2}-(w_{j+1}^n+w_j^n)/2}{\Delta t/2}+a\frac{w_{j+1}^n-w_j^n}{\Delta x}=0$ $\frac{w_j^{n+1}-w_j^n}{\Delta t}-a\frac{w_{j+1/2}^{n+1/2}-w_{j-1/2}^{n+1/2}}{\Delta x}=0$	Same as Lax-Wendroff I	Stable for $\dot{a}\leq 1$
MacCormack  (Predictor/Corrector)	$\frac{w_j^t-w_j^n}{\Delta t}+a\frac{w_{j+1}^n-w_j^n}{\Delta x}=0$ $\frac{w_j^{n+1}-(w_j^n+w_j^t)/2}{\Delta t}+a\frac{w_j^t-w_{j-1}^t}{\Delta x}=0$	Same as Lax-Wendroff I	Stable for $\dot{a}\leq 1$
Beam-Warming  (Predictor/Corrector)	$\frac{w_j^{n+1}-w_j^n}{\Delta t}+a\frac{3w_j^n-4w_{j-1}^n+w_{j-2}^n}{2\Delta x}$ $-\frac{a^2\Delta t}{2\Delta x^2}(w_j^n-2w_{j-1}^n+w_{j-2}^n)=0$	$\frac{a\Delta x^2}{6}(1-\dot{a})(2-\dot{a})w_{xxx}$ $-\frac{a\Delta x^3}{8}(1-\dot{a})^2(2-\dot{a})w_{xxxx}$	Stable for $0\leq\dot{a}\leq 2$
QUICK 	$\frac{w_j^{n+1}-w_j^n}{\Delta t}+a\frac{(3w_j^n+6w_{j-1}^n-w_{j-2}^n)-(3w_{j+1}^n+6w_j^n-w_{j-1}^n)}{8\Delta x}=0$		Stable for $\dot{a}\leq 1$

Stability in terms of fluxes: FTCS for Advection

Consider $\boxed{\dfrac{\partial w}{\partial t} + \dfrac{\partial F}{\partial x} = 0}$ with $F = aw$

- Finite volume approximation:

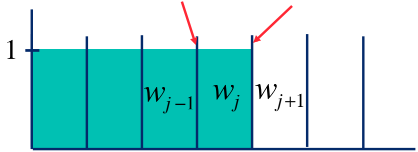
$$\frac{dw_j}{dt} = \frac{F_{j-\frac{1}{2}} - F_{j+\frac{1}{2}}}{\Delta x} \qquad F_{j+\frac{1}{2}} = aw_{j+\frac{1}{2}} \approx \frac{a}{2}(w_{j+1}+w_j)$$

- Update:

$$w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x}(F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}})$$
$$= w_j^n - \frac{a\Delta t}{2\Delta x}(w_{j+1} - w_{j-1})$$

- Consider the following IC with a=1 and $\dfrac{\Delta t}{\Delta x}$=0.5:

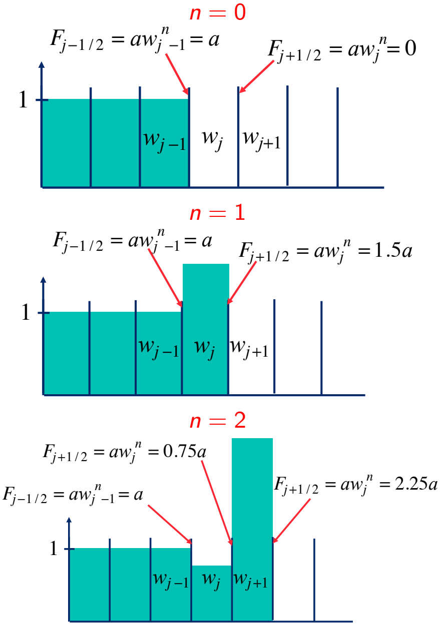
$$F_{j-\frac{1}{2}}=\frac{a}{2}(w^n_{j-1} + w^n_j)=1 \qquad F_{j+\frac{1}{2}}=\frac{a}{2}(w^n_{j+1} + w^n_j)=0.5$$



$$w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x}(F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}})$$
$$= 1 - 0.5 \cdot (0.5 - 1) = 1.25$$

- **Cell j will overflow immediately!**
- It is easy to see why the centred difference approximation is always unstable

Stability in terms of Fluxes: Upwind for Advection



- Finite volume approximation:

$$\frac{dw_j}{dt} = \frac{F_{j-\frac{1}{2}} - F_{j+\frac{1}{2}}}{\Delta x} \qquad F_{j+\frac{1}{2}} = aw_{j+\frac{1}{2}} \approx aw_j$$

- Update:

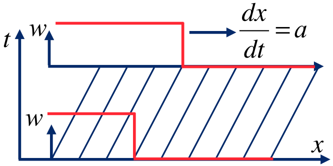
$$w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x}\Big(\overbrace{F_{j+\frac{1}{2}}^n}^{=aw_{j-1}^n} - \overbrace{F_{j-\frac{1}{2}}^n}^{=aw_j^n}\Big) = w_j^n - \frac{a\Delta t}{\Delta x}(w_j^n - w_{j-1}^n)$$

- Consider $a = 1$, $\frac{\Delta t}{\Delta x} = 1.5a = 1.5$. Start iterations:
  - $n = 0$: $\quad w_j^0 = 0 \qquad F_{j+\frac{1}{2}}^0 = 0 \qquad F_{j-\frac{1}{2}}^0 = 1$
  - $n = 1$:
  $$w_j^1 = w_j^0 - \frac{\Delta t}{\Delta x}\left(F_{j+\frac{1}{2}}^0 - F_{j-\frac{1}{2}}^0\right) = 0 - 1.5 \cdot (0 - 1) = 1.5$$
  - $n = 2$:
  $$w_j^2 = w_j^1 - \frac{\Delta t}{\Delta x}\left(F_{j+\frac{1}{2}}^1 - F_{j-\frac{1}{2}}^1\right) = 0 - 1.5 \cdot (1.5 - 1) = 0.75$$
  $$w_{j+1}^2 = w_{j+1}^1 - \frac{\Delta t}{\Delta x}\left(F_{j+\frac{3}{2}}^1 - F_{j+\frac{1}{2}}^1\right) = 0 - 1.5 \cdot (0 - 1.5) = 2.25$$
  - $n = 3$: Even larger positive value, until overflow (NaN)
    - If $\frac{a\Delta t}{\Delta x} > 1$ scheme unstable!

Discontinuous solutions: shocks

Linear advection Equation

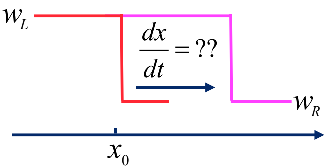
$$\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = 0 \quad w(x,0) = \begin{cases} w_L & x < x_0 \\ w_R & x > x_0 \end{cases} \qquad (w_L > w_R)$$



- Analytic solution obtained by characteristics: $\frac{\mathrm{d}x}{\mathrm{d}t} = a \qquad \frac{\mathrm{d}w}{\mathrm{d}t} = 0$
- Discontinuity of solution is allowed!

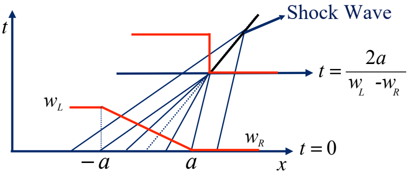
Inviscid Burgers' Equation

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial x} = 0 \quad w(x,0) = \begin{cases} w_L & x < x_0 \\ w_R & x > x_0 \end{cases} \qquad (w_L > w_R)$$



- Characteristics: $\frac{\mathrm{d}x}{\mathrm{d}t} = w \qquad \frac{\mathrm{d}w}{\mathrm{d}t} = 0$
- Slight variation of the initial condition: formation of shock

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

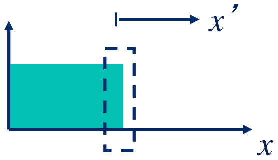


- How to compute the shock speed?

Shock speed

Reference frame of the shock: $x' = x - Ct$

$$\Longrightarrow \quad \frac{\partial w}{\partial t} = \frac{\partial w}{\partial t} + \frac{\partial w}{\partial x'}\frac{\partial x'}{\partial t} = \frac{\partial w}{\partial t} + C\frac{\partial w}{\partial x'}$$



Replace into the equation:

$$\frac{\partial w}{\partial t} + \frac{\partial F}{\partial x} = 0$$

$$\frac{\partial w}{\partial t} - C\frac{\partial w}{\partial x'} + \frac{\partial F}{\partial x'} = 0$$

$$\int_{\Delta\to 0}\left(\frac{\partial w}{\partial t} - C\frac{\partial w}{\partial x'} + \frac{\partial F}{\partial x'}\right)\mathrm{d}x = 0$$

$$\cancel{\int_{\Delta\to 0}\frac{\partial w}{\partial t}\mathrm{d}x} - \int_{\Delta\to 0} C\frac{\partial w}{\partial x'}\mathrm{d}x + \int_{\Delta\to 0}\frac{\partial F}{\partial x'}\mathrm{d}x = 0$$

$$-C(w_R - w_L) + (F_R - F_L) = 0$$

- **Rankine-Hugoniot Relations!**

$$\boxed{C = \frac{F_R - F_L}{w_R - w_L}}$$

Example:

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

$$C = \frac{F_R - F_L}{w_R - w_L} = \frac{1}{2}\frac{w_R^2 - w_L^2}{w_R - w_L}$$

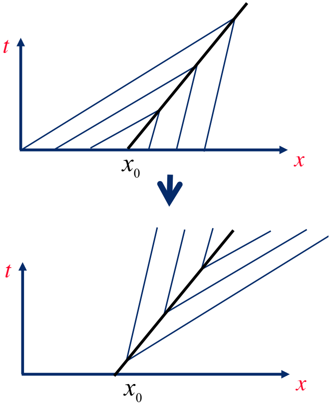
$$= \frac{1}{2}\frac{(w_R + w_L)\cdot\cancel{(w_R - w_L)}}{\cancel{w_R - w_L}}$$

$$= \frac{1}{2}(w_R - w_L)$$

Entropy conditions (I)

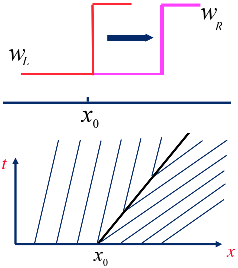
Inviscid Burgers equation: $\boxed{\dfrac{\partial w}{\partial t} + w\dfrac{\partial w}{\partial x} = 0}$ **Characteristics:** $\dfrac{\mathrm{d}x}{\mathrm{d}t} = w, \quad \dfrac{\mathrm{d}w}{\mathrm{d}t} = 0$

- The transformation $x \to -x$, $t \to -t$ leaves the equation unchanged but results in unphysical solution!
- Need for entropy condition to select the correct one

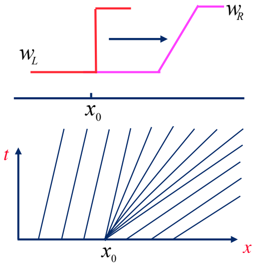


Consider $w(x,0) = \begin{cases} w_L & x < x_0 \\ w_R & x > x_0 \end{cases} \qquad (w_L < w_R)$

Reverse shock (?)
Unstable, entropy-violating solution



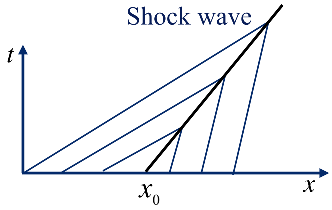
Rarefaction wave
Physically correct solution



Entropy conditions (II)

Weak solution to hyperbolic equations may not be unique

- How to find the **physical solution** out of many weak solution?
- The actual physics always includes **dissipation**: $\dfrac{\partial w}{\partial t} + w\dfrac{\partial w}{\partial x} = \nu \dfrac{\partial^2 w}{\partial x^2}$
  - What we are seeking is the solution for viscous Burgers' eq. for $\nu \to 0$



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

$$(I) \qquad F'(w_L) > C > F'(w_R)$$

$$(II) \qquad \frac{F(w) - F(w_L)}{w - w_L} \geq C \geq \frac{F(w) - F(w_R)}{w - w_R} \quad \text{for} \quad w_L \geq w \geq w_R$$

Given $\dfrac{\partial w}{\partial t} + \dfrac{\partial F(w)}{\partial x} = 0$, in characteristic form:

$$\frac{\partial w}{\partial t} + \frac{\partial F}{\partial w}\frac{\partial w}{\partial x} = 0 \quad \text{where} \quad \frac{dt}{ds} = 1, \quad \frac{dx}{ds} = \frac{\partial F}{\partial w} \quad \Longrightarrow \quad \frac{dx}{dt} = \frac{\partial F}{\partial w} = F'(w)$$

- The condition states that characteristics must "enter" the discontinuity $\Longrightarrow$ its speed C must satisfy (I)
- Since $C = \dfrac{F_R - F_L}{w_R - w_L}$, then (II) is satisfied
  - The hypothetical shock speed for values of w between L and R must give shock speeds that are larger on the left and smaller on the right

Conservative discretization

In FVM, equations in **conservative forms** are needed in order to satisfy conservation properties!

- Consider a 1D equation

$$\frac{\partial w}{\partial t} + \frac{\partial F[w(x,t)]}{\partial x} = 0 \qquad x \in [0, L]$$

with F a general advection or diffusion term

- Integrate over the domain L:

$$\int_0^L \frac{\partial w}{\partial t}\,\mathrm{d}x + \cancel{\int_0^L \frac{\partial F}{\partial x}}\,\mathrm{d}x = 0$$

$$F(L) - F(0) = 0 \implies \frac{\mathrm{d}}{\mathrm{d}t}\int_L w\,\mathrm{d}x = 0$$

  - If $F = 0$ at the endpoints, w is conserved!

- In discretized form:

$$\int_0^L \frac{\partial F}{\partial x}\,\mathrm{d}x = \sum \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\cancel{\Delta x}}\cancel{\Delta x}$$

$$= [..+F_{j-\frac{1}{2}} - F_{j-\frac{3}{2}} + F_{j+\frac{1}{2}}$$

$$- F_{j-\frac{1}{2}} + F_{j+\frac{3}{2}} - F_{j+\frac{1}{2}} + ..]$$

$$= F_L - F_0$$

Examples: $\dfrac{\partial\left(\frac{1}{2}w^2\right)}{\partial x}$ vs $w\dfrac{\partial w}{\partial x}$

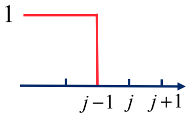
$$\underbrace{\frac{\partial\left(\frac{1}{2}w^2\right)}{\partial x}}_{=} \approx \underbrace{\frac{1}{2\Delta x}\left(w_j^2 - w_{j-1}^2\right)}_{\neq} \qquad \textbf{Cons.}$$

$$\overbrace{w\frac{\partial w}{\partial x}} \approx \overbrace{\frac{w_j}{\Delta x}\left(w_j - w_{j-1}\right)} \qquad \textbf{Non cons.}$$

- Terms cancel out only for conservative form!
  - Cons. schemes guarantee the correct shock speed
  - Non-cons. schemes may or may not. Example:

$$\textbf{(NC)} \quad w_j^{n+1} = w_j^n - \frac{\Delta t}{\Delta x} w_j^n\left(w_j^n - w_{j-1}^n\right) = 0$$

$$\textbf{(C)} \quad w_j^{n+1} = w_j^n - \frac{\Delta t}{2\Delta x}\left[\left(w_j^n\right)^2 - \left(w_{j-1}^n\right)^2\right] = \frac{\Delta t}{2\Delta x}$$



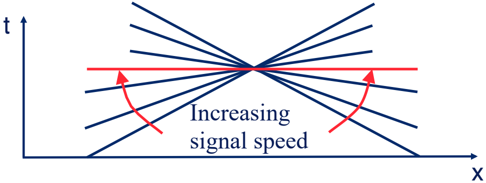
With **(NC)**, shock never moves!

1D heat equation: explicit method

$$\boxed{\frac{\partial w}{\partial t} = \nu \frac{\partial^2 w}{\partial x^2}}, \qquad t > 0, a \le x \le b$$

Parabolic equation requiring

- **Initial Condition**: $w(x,0) = w_0(x)$
- **Boundary Conditions**:
  - Dirichlet: $w(a,t) = \phi_a(t)$
  - Neumann: $\frac{\partial w}{\partial x}(a,t) = \varphi_a(t)$



- Can be viewed as the limit of a hyperbolic equation as signal speed $\to \infty$
- **Example of explicit method**: **FTCS**

$$\frac{w_j^{n+1} - w_j^n}{\Delta t} = \nu \frac{w_{j+1}^n - 2w_j^n + w_{j-1}^n}{\Delta x^2}$$

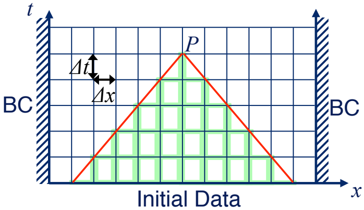
- **Modified equation**:

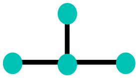
$$\frac{\partial w}{\partial t} - \nu \frac{\partial^2 w}{\partial x^2} = \frac{\nu \Delta x^2}{12}(1 - 6\dot{\nu}) w_{xxxx} + \mathcal{O}(\Delta t^2, \Delta x^2 \Delta t, \Delta x^4) w_{6x} \quad \text{with} \quad \dot{\nu} = \frac{\nu \Delta t}{\Delta x^2}$$

  - Accuracy $\mathcal{O}(\Delta t, \Delta x^2)$
- **Stability analysis** gives the **Fourier condition**:

$$G = \frac{\widehat{w}^{n+1}}{\widehat{w}^n} = 1 - 4\frac{\nu \Delta t}{\Delta x^2} \sin^2 k \frac{\Delta x}{2} = 1 - 4\dot{\nu} \sin^2 \frac{\beta}{2}$$

$$\implies -1 < 1 - 4\dot{\nu} < 1 \iff 0 \le \dot{\nu} \le \frac{1}{2}$$





- Boundary effect not felt at P for many time steps with FTCS! May result in unphysical behavior

1D heat equation: implicit method

- Example of **implicit method**: **Backward Euler**

$$\frac{w_j^{n+1} - w_j^n}{\Delta t} = \nu \frac{w_{j+1}^{n+1} - 2w_j^{n+1} + w_{j-1}^{n+1}}{\Delta x^2}$$

- **Modified equation**:

$$\frac{\partial w}{\partial t} - \nu \frac{\partial^2 w}{\partial x^2} = \frac{\nu \Delta x^2}{12}(1+6\dot{\nu})w_{4x} + \mathcal{O}(\Delta t^2, \Delta x^2 \Delta t, \Delta x^4)w_{6x}$$

  - The $+$ sign suggests that implicit methods may be less accurate than corresponding explicit ones

- **Stability analysis**:

$$G = \frac{\widehat{w}^{n+1}}{\widehat{w}^n} = \frac{1}{1 + 2\dot{\nu}(1 - \cos\beta)}$$

  - Unconditionally stable!

- Rewritten as a tridiagonal matrix system:

$$w_j^{n+1} - w_j^n = \frac{\nu \Delta t}{\Delta x^2}(w_{j+1}^{n+1} - 2w_j^{n+1} + w_{j-1}^{n+1})$$

$$\dot{\nu} w_{j-1}^{n+1} - (1 + 2\dot{\nu}) w_j^{n+1} + \dot{\nu} w_{j+1}^{n+1} = -w_j^n$$

$$a_k w_{k-1} - d_k w_k + c_k w_{k+1} = b_k$$

- Write in matrix form:

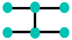
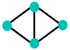
$$\begin{aligned}
d_1 w_1 + c_1 w_2 \quad & = b_1 \\
a_2 w_1 + d_2 w_2 \quad + c_2 w_3 \quad & = b_2 \\
\ddots \quad & \\
a_{N-1} w_{N-2} + d_{N-1} w_{N-1} + c_{N-1} w_N & = b_{N-1} \\
a_N w_{N-1} + \quad d_N w_N & = b_N
\end{aligned}$$

If endpoints are given: $b_1 = -a_1 w_0$, $b_N = -c_N w_{N+1}$

- Linear system to be solved

Summary

$$\boxed{\frac{\partial w}{\partial t} + \nu \frac{\partial^2 w}{\partial x^2} = 0} \qquad \dot{\nu} = \frac{\nu \Delta t}{\Delta x^2}$$

Name / Stencil	Scheme	Error term	Stability
FTCS 	$\frac{w_j^{n+1} - w_j^n}{\Delta t} = \nu \frac{w_{j+1}^n - 2w_j^n + w_{j-1}^n}{\Delta x^2}$	$\frac{\nu \Delta x^2}{12}(1 - 6\dot{\nu}) w_{4x}$	Stable for $\dot{\nu} \leq \frac{1}{2}$
BTCS 	$\frac{w_j^{n+1} - w_j^n}{\Delta t} = \nu \frac{w_{j+1}^{n+1} - 2w_j^{n+1} + w_{j-1}^{n+1}}{\Delta x^2}$	$\frac{\nu \Delta x^2}{12}(1 + 6\dot{\nu}) w_{4x}$	Unconditionally Stable
Crank-Nicolson 	$\frac{w_j^{n+1} - w_j^n}{\Delta t} = \frac{\nu}{2\Delta x^2}\Big[(w_{j+1}^{n+1} - 2w_j^{n+1} + w_{j-1}^{n+1}) + (w_{j+1}^n - 2w_j^n + w_{j-1}^n)\Big]$	$\frac{\nu \Delta x^2}{12} w_{4x} + \frac{\nu^3 \Delta t^2}{12} w_{6x}$	Unconditionally Stable
DuFort-Frankel 	$\frac{w_j^{n+1} - w_j^{n-1}}{2\Delta t} = \nu \frac{(w_{j+1}^n - w_j^{n+1} - w_j^{n-1} + w_{j-1}^n)}{\Delta x^2}$	$\frac{\nu \Delta x^2}{12}(1 - 12\dot{\nu}^2) w_{4x}$	Unconditionally Stable, Conditionally consistent

$$\frac{w_j^{n+1} - w_j^n}{\Delta t} = \nu \left[\theta \frac{w_{j+1}^{n+1} - 2w_j^{n+1} + w_{j-1}^{n+1}}{\Delta x^2} + (1-\theta) \frac{w_{j+1}^n - 2w_j^n + w_{j-1}^n}{\Delta x^2}\right] \qquad \theta = \begin{cases} 0 & \text{Explicit (FTCS)} \\ 1 & \text{Implicit (BTCS)} \\ 1/2 & \text{Crank-Nicolson} \end{cases}$$

Stability in terms of fluxes: FTCS for Diffusion

Consider $\boxed{\dfrac{\partial w}{\partial t} + \dfrac{\partial F}{\partial x} = 0}$ with $F = -\nu \dfrac{\partial w}{\partial x}$

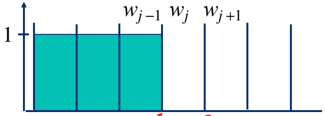
- Finite volume approximation:

$$\frac{dw_j}{dt} = \frac{F_{j-\frac{1}{2}} - F_{j+\frac{1}{2}}}{\Delta x} \qquad F_{j+\frac{1}{2}} = -\nu \frac{w_{j+1} - w_j}{\Delta x}$$

- Update:

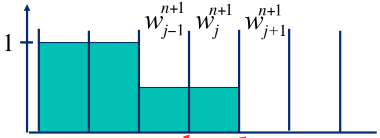
$$w_j^{n+1} = w_j^n + \frac{\nu \Delta t}{\Delta x^2}(w_{j+1}^n - 2w_j^n - w_{j-1}^n)$$

- Consider the following initial conditions:



$$F_{j-\frac{1}{2}} = -\nu \frac{w_j - w_{j-1}}{\Delta x} = \frac{\nu}{\Delta x} \qquad F_{j+\frac{1}{2}} = -\nu \frac{w_{j+1} - w_j}{\Delta x} = 0$$

- $\dfrac{\nu \Delta t}{\Delta x}$ of w flows into cell j, but nothing flow out
- Eventually, cell $j-1$ becomes empty and j full..



$$F_{j-\frac{1}{2}} = \frac{\nu}{\Delta x} \qquad F_{j+\frac{1}{2}} = 0$$

- It seems reasonable to limit Δt such that we stop when both cells are equally full

$$w_{j-1}^n + \frac{\nu \Delta t}{\Delta x^2}(w_j^n - 2w_{j-1}^n + w_{j-2}^n)$$
$$= w_j^n + \frac{\nu \Delta t}{\Delta x^2}(w_{j+1}^n - 2w_j^n + w_{j-1}^n)$$

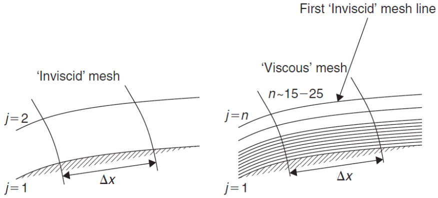
Since $w_{j-2}^n = w_{j-1}^n = 1$ and $w_j^n = w_{j+1}^n = 0$ we get:

$$1 + \frac{\nu \Delta t}{\Delta x^2}(0 - 2 + 1) = 0 + \frac{\nu \Delta t}{\Delta x^2}(0 - 0 + 1)$$

- Or $\dfrac{\nu \Delta t}{\Delta x^2} = 2$ as maximum value for stability!

Grid requirements for BLs

- BLs have dramatic consequences on grid requirements:
  - Thickness of the order of $1/\sqrt{Re}$
  - Need for a minimum of 10-20 points in the BL: **clustering** of the grid points close to the wall



Model problem for BLs:
advection-diffusion equation

$$\boxed{\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = \nu\frac{\partial^2 w}{\partial x^2}}$$

Consider the steady-state **model problem** (2-point BVP)

$$a\frac{\partial w}{\partial x} = \nu\frac{\partial^2 w}{\partial x^2} \quad \text{with} \quad w \in [0, L], \quad w(0) = \alpha, \quad w(L) = \beta$$

- Define $Re_u = \dfrac{a}{\nu} \quad \Longrightarrow \quad (\star)\dfrac{\partial^2 w}{\partial x^2} - Re_u\dfrac{\partial w}{\partial x} = 0$

$$\Longrightarrow \begin{cases} Re_u \ll 1 & \text{heat equation, easy to solve} \\ Re_u = \mathcal{O}(1) & \text{usual advection-diffusion eq} \\ Re_u \gg 1 & \textbf{problem!} \end{cases}$$

- As $1/Re_u \to 0$:
  - **Singularly perturbed eq.**: small perturbations change the behaviour
  - $(\star)$ reduces to 1^{st}-order (**Overimposed problem**)
  - $w(x)$ tends to discontinuous function that jumps to β
  - Region of strong transition called boundary layer of thickness $\mathcal{O}(1/Re)$
- **Analytical solution**:

$$w(x) = \alpha + (\beta - \alpha)\frac{\exp\left[\frac{ax}{\nu}\right] - 1}{\exp\left[\frac{aL}{\nu}\right] - 1} = \alpha + (\beta - \alpha)\frac{\exp(Re_x) - 1}{\exp(Re_L) - 1}$$

Preliminary considerations

- Simplest case: $\alpha = 0$, $\beta = 1$:

$$\boxed{w(x) = \frac{\exp(Re_x) - 1}{\exp(Re_L) - 1}}$$

- Suppose to represent the **exact** solution on a discrete mesh, defined as $x_j = j\Delta x$ with $j \in [1, N]$:

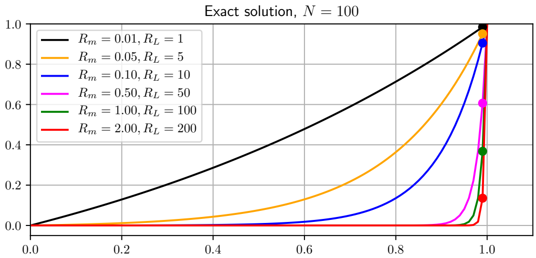
$$Re_x = \frac{ax}{\nu} = \frac{aj\Delta x}{\nu} = jR_m$$

$$Re_L = \frac{aL}{\nu} = \frac{aN\Delta x}{\nu} = NR_m$$

$$\implies \quad w_j = \frac{e^{jR_m} - 1}{e^{NR_m} - 1}$$

$$w_{N-1} = \frac{e^{(N-1)R_m} - 1}{e^{NR_m} - 1} = \frac{1}{e^{R_m}} \quad \text{for} \quad N \gg 1$$

  - w_{N-1} vanishes quickly for $R_m > 1$: the boundary layer is no longer resolved
  - Similar problems for interior layers



- $R_m = \dfrac{|a|\Delta x}{\nu}$ is the **Mesh Reynolds number**
  - Ratio of the time needed to **advect** the solution over one cell to the time needed to **diffuse** it

Now let's try to solve the **discretized equation**

- Transport phenomena intrinsically isotropic $\implies$ no physical reason for upwinding viscous terms
- Try using 1st-order (upwind) or 2nd-order (centred) scheme for convective term

The Advection-Diffusion equation - Upwind

Recall the operators δ and μ:

$$\delta(\bullet)_{j+\frac{1}{2}} = (\bullet)_{j+1} - (\bullet)_j$$

$$\mu(\bullet)_{j+\frac{1}{2}} = \frac{1}{2}\left[(\bullet)_{j+1} + (\bullet)_j\right]$$

$$\delta\mu(w)_j = \delta\left[\frac{1}{2}\left(w_{j+\frac{1}{2}} + w_{j-\frac{1}{2}}\right)\right]$$

$$= \frac{1}{2}\left[(w_{j+1} - w_j) + (w_j - w_{j-1})\right] = \frac{w_{j+1} - w_{j-1}}{2}$$

$$\delta^2(w)_j = \delta\left[w_{j+\frac{1}{2}} - w_{j-\frac{1}{2}}\right]$$

$$= \left[w_{j+1} - w_j - (w_j - w_{j-1})\right] = w_{j+1} - 2w_j + w_{j-1}$$

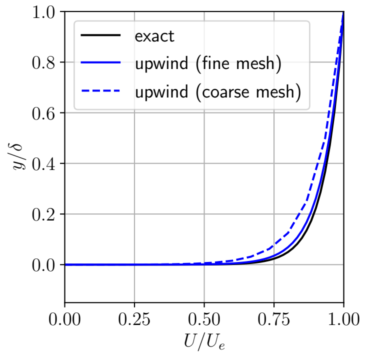
Generalized Upwind:

(sum of centred term + numerical dissipation):

$$\frac{w_j^{n+1} - w_j^n}{\Delta t} + a\frac{\delta\mu w_j^n}{\Delta x} - \frac{1}{2}|a|\Delta x\left[\frac{\delta^2 w_j^n}{\Delta x^2}\right] = \nu\frac{\delta^2 w_j^n}{\Delta x^2}$$

$$\frac{w_j^{n+1} - w_j^n}{\Delta t} + a\frac{\delta\mu w_j^n}{\Delta x} = \nu\left[1 + \frac{R_m}{2}\right]\frac{\delta^2 w_j^n}{\Delta x^2}$$

Velocity profile inside a BL



- Numerical diffusion **adds** to the physical one
- Computed velocity profiles correspond to a **lower** *Re* than the physical one
- Possible solutions:
  - Use finer grids (costly)
  - Use a centred (non-dissipative) scheme

The Advection-Diffusion equation - FTCS (I)

FTCS:

$$\frac{w_j^{n+1}-w_j^n}{\Delta t}+a\frac{w_{j+1}^n-w_{j-1}^n}{2\Delta x}=\nu\frac{w_{j+1}^n-2w_j^n+w_{j-1}^n}{\Delta x^2}$$

- **Modified equation**:

$$\frac{\partial w}{\partial t}+a\frac{\partial w}{\partial x}=\left(\nu-\frac{a^2\Delta t}{2}\right)\frac{\partial^2 w}{\partial x^2}-\frac{a\Delta x^2}{6}\frac{\partial^3 w}{\partial x^3}+\mathcal{O}(\Delta x^3,\Delta t^2)$$

- **Von Neumann analysis**:

$$\frac{\widehat{w}_j^{n+1}-\widehat{w}_j^n}{\Delta t}+a\frac{\widehat{w}_{j+1}^n-\widehat{w}_{j-1}^n}{\Delta x}=\nu\frac{\widehat{w}_{j+1}^n-2\widehat{w}_j^n+\widehat{w}_{j-1}^n}{\Delta x^2}$$

$$\begin{aligned}G&=1-\frac{a\Delta t}{2\Delta x}\left(e^{i\beta}-e^{-i\beta}\right)+\frac{\nu\Delta t}{\Delta x^2}\left(e^{i\beta}-2+e^{-i\beta}\right)\\&=1-2\dot{\nu}(1-\cos\beta)-i\dot{a}\sin\beta\\&=1-4\dot{\nu}\sin^2\frac{\beta}{2}-2i\dot{a}\sin\frac{\beta}{2}\cos\frac{\beta}{2}\end{aligned}$$

1. $\widehat{w}_{j\pm1}^n=\widehat{w}^n e^{ikx_j}e^{\pm ik\Delta x}$
2. $e^{\pm ik\Delta x}=e^{\pm i\beta}=\cos\beta\pm i\sin\beta$

Rename $\frac{\beta}{2}=\xi$. For stability, $|G|^2\le 1$:

$$1-8\dot{\nu}\sin^2\xi+16\dot{\nu}^2\sin^4\xi+4\dot{a}\sin^2\xi\cos^2\xi\le 1$$

$$8\dot{\nu}\sin^2\xi(2\dot{\nu}\sin^2\xi-1)+4\dot{a}^2\sin^2\xi\cos^2\xi\le 0$$

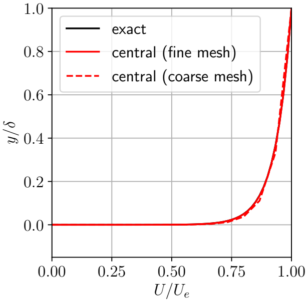
$$\underbrace{\frac{\dot{\nu}}{\dot{a}^2}\frac{2}{\cos^2\xi}\Big(\overbrace{2\dot{\nu}\sin^2\xi-1}^{\text{must be}\le 0}\Big)}_{\text{must be}\le -1}+1\le 0$$

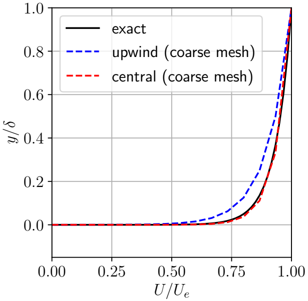
$$2\dot{\nu}\le 1 \quad\text{and}\quad 2\dot{\nu}\ge\dot{a}^2$$

$$\Delta t\le\frac{\Delta x^2}{2\nu}\quad\text{and}\quad\Delta t\le\frac{2\nu}{a^2}$$

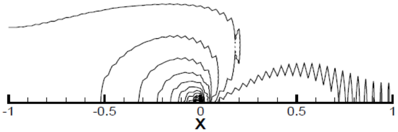
- It was unconditionally unstable for pure advection
  - Physical diffusion stabilises the centred scheme
- Red limit from heat equation
- Blue limit may also be derived from the modified equation (positive dissipation term)
  - Defining $R_m=\frac{a\Delta x}{\nu}$, one has: $R_m\le\frac{2}{\dot{a}}$

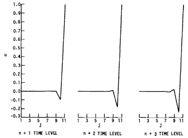
The Advection-Diffusion equation - FTCS (II)





- It is possible to prove that oscillating solutions are obtained if $R_m > 2$!





- Re-write the scheme under the form:

$$w_j^{n+1} = \left(\dot{\nu} - \frac{\dot{a}}{2}\right) w_{j+1}^n + (1 - 2\dot{\nu}) w_j^n + \left(\dot{\nu} + \frac{\dot{a}}{2}\right) w_{j-1}^n$$
$$= \frac{\dot{\nu}}{2}(2 - R_m) w_{j+1}^n + (1 - 2\dot{\nu}) w_j^n + \frac{\dot{\nu}}{2}(2 + R_m) w_{j-1}^n$$

- Suppose $w^0 = 0$ everywhere (apart for $w_N^0 = 1$ at $j = N$ for B.C.)

$$w_{N-1}^1 = \frac{\dot{\nu}}{2}(2 - R_m) w_N^0 + (1 - 2\dot{\nu}) w_{N-1}^0 + \frac{\dot{\nu}}{2}(2 + R_m) w_{N-2}^0$$

  - if $R_m > 2 \implies w_{N-1}^1 < 0 \implies$ **oscillations!**
  - This becomes worst at subsequent time levels
  - Thus, fine grids again... or **compromise solution**:
    - Add numerical diss. as smaller as possible (given stab. requirements)
    - High-order dissipative schemes well suited (e.g, 2nd-order upwind)

The Advection-Diffusion equation - Summary

$$\boxed{\frac{\partial w}{\partial t} + a\frac{\partial w}{\partial x} = \nu \frac{\partial^2 w}{\partial x^2}}$$

Upwind

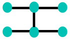
$$w_j = \frac{1-(1+R_m)^j}{1-(1+R_m)^N}$$

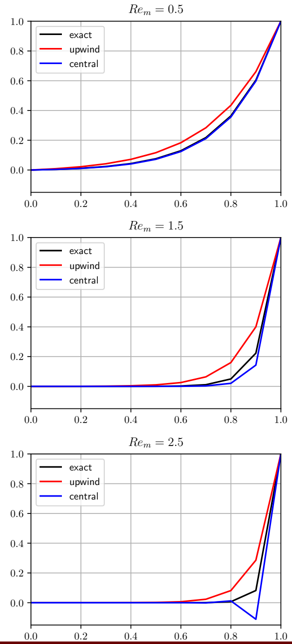
Centred

$$w_j = \frac{\left(\dfrac{2+R_m}{2-R_m}\right)^j - 1}{\left(\dfrac{2+R_m}{2-R_m}\right)^N - 1}$$

Exact

$$w_j = \frac{e^{jR_m}-1}{e^{NR_m}-1}$$

Name / Stencil	Error term	Stability
FTCS 	$\mathcal{O}(\Delta t, \Delta x^2)$	$\dot\nu \le \frac{1}{2}$ & $\dot\nu \ge \frac{\dot a^2}{2}$
Upwind 	$\mathcal{O}(\Delta t, \Delta x)$	$\dot a + 2\dot\nu \le 1$
Lax-Wendroff 	$\mathcal{O}(\Delta t^2, \Delta x^2)$	$\dot a^2 \le 2\dot\nu \le 1$
Crank-Nicolson 	$\mathcal{O}(\Delta t^2, \Delta x^2)$	Unconditionally stable



Complexity for discretization of RANS equations

- **Time step**:

$$\Delta t = \min(\Delta t_c, \Delta t_v) \quad \text{with} \begin{cases} \Delta t_c = \mathcal{O}\left(\dfrac{\Delta x}{|u| + a}\right) \\ \Delta t_v = \mathcal{O}\left(\dfrac{\Delta x^2}{\nu}\right) \end{cases} \implies \frac{\Delta t_v}{\Delta t_c} = \mathcal{O}\left(\frac{(|u| + a)\Delta x}{\nu}\right) = \mathcal{O}\left[R_m\left(1 + \frac{1}{Ma}\right)\right]$$

  - For low-Ma flows, $\Delta t_v \gg \Delta t_c$; the opposite for high-$Ma$ flows
  - Small grid size near the wall $\implies$ explicit schemes **costly** because of viscous terms
    - **Implicit schemes** relax the constraint but require efficient solution of linear systems at each iteration

- **Turbulent transport equations**
  - **Numerical stiffness** introduced by source terms
  - **Strong coupling** of equations by means of source and diffusion terms
  - Problems related to the need of preserving **variable positiveness**
    - Crucial point to avoid the use of brutal limiters damaging the solution convergence

- **Discretization of convective terms**
  - 1st-order upwind schemes?
    - ✔ Ensure positivity of variables
    - ✘ Low accuracy!
  - TVD schemes?
    - ✔ Ensure positivity of variables
    - ✘ Difficult to develop schemes that are TVD and implicit at the same time (Needed for using large CFL on stretched grids)
  - Positivity-preserving, not-TVD schemes?
  - ✔ Ensure positivity of variables
  - ✘ Oscillations near discontinuities