Numerical methods for 1st order wave equation: $\partial_t f + a\,\partial_x f = 0$

A. Euler explicit $(f^{n+1} - f^n)/\Delta t = -a\,\delta_x f^n$

1. Central (FTCS)

$$(f_j^{n+1} - f_j^n) = -a\,\Delta t/2\Delta x\,(f_{j+1}^n - f_{j-1}^n) = -C/2\,(f_{j+1}^n - f_{j-1}^n)$$

$$f_j^{n+1} = f_j^n - C/2\,(f_{j+1}^n - f_{j-1}^n)$$

$C = a\,\Delta t/\Delta x$ is Courant-Fredrichs-Lewy (CFL) number.

VonNeuman stability: $\varepsilon_j^{n+1} = \varepsilon_j^n - C/2\,(\varepsilon_{j+1}^n - \varepsilon_{j-1}^n)$. Error is of form $\varepsilon^n = A^n e^{i\Theta j}$:

$$A^{n+1} = A^n[1 - C/2\,(e^{i\Theta} - e^{-i\Theta})] = A^n[1 - iC\sin\Theta]$$

Amplification factor:

$$G = \|A^{n+1}/A^n\| = \|1 - iC\sin\Theta\| = \sqrt{1+C^2\sin^2\Theta} \geq 1$$

Unconditionally unstable   Max growth @ $\pi/2$

2. One sided difference for $-a\,\partial_x f^n$

Assume that $C > 0$

$$(f_j^{n+1} - f_j^n) = \underbrace{-C\,(f_{j+1}^n - f_j^n)}_{downwind} \quad \text{or} = \underbrace{-C\,(f_j^n - f_{j-1}^n)}_{upwind}$$

$$f_j^{n+1} = f_j^n - C\,(f_{j+1}^n - f_j^n) \;;\quad f_j^n - C\,(f_j^n - f_{j-1}^n)$$

$A^{n+1} = A^n[1 - C\,(e^{i\Theta} - 1)]$ downwind

$A^{n+1} = A^n[1 - C\,(1 - e^{-i\Theta})]$ upwind

case 1 (downwind)
$$\begin{aligned} G^2 &= (1+C-C\cos\Theta)^2 + C^2\sin^2\Theta \\ &= (1+C)^2 - 2(C+C^2)\cos\Theta + C^2 \\ &= 1+2C+2C^2-2(C+C^2)\cos\Theta \\ &= 1+2(C^2+C)(1-\cos\Theta) > 1 \end{aligned}$$

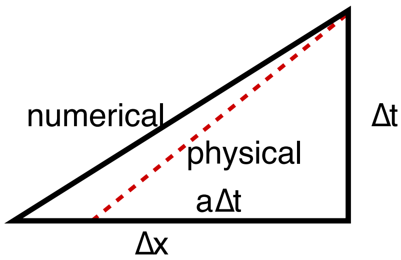
case 2 (upwind)
$$\begin{aligned} G^2 &= (1 - C + C\cos\Theta)^2 + C^2\sin^2\Theta \\ &= (1 - C)^2 + 2(C-C^2)\cos\Theta + C^2 \\ &= 1 - 2C + 2C^2 - 2(C^2 - C)\cos\Theta \\ &= 1+2(C^2-C)\,\underbrace{(1-\cos\Theta)}_{\geq 0} \end{aligned}$$

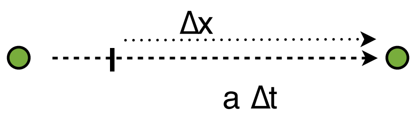
$G<1$ if $C^2 - C < 0 \rightarrow \boxed{0 < C < 1}$ ∴ Upwind

Upwind is stable if CFL<1; or $\Delta t < \Delta x/a$. *Downwind* is unstable! (C=1 has no error, but this is not useful)

Animations: *Convect_exact.gif, Convect_Central.gif, Convect_Up.gif,exact.giRK_central.gif*

B. Physical interpretations:





a. Convection is from upwind, not down. If $a<0$ upwind is other direction (*j+1*).

b. In one time-step, particle can't move more than the stencil (receiving grid point won't have info): $a\Delta t < \Delta x$ -> $C = a\Delta t/\Delta x < 1$.

c. Numerical domain of dependence must include physical domain of dependence. Stable if physical $\subset$ numerical. Unstable if numerical $\subset$ physical.

1. Another view of upwinding: numerical viscosity: upwind = central + diffusion

$$\delta f/\delta t = -a/\Delta x(f_j - f_{j-1}) = -a/(2\Delta x)(f_{j+1} - f_{j-1}) + a/(2\Delta x)(f_{j+1} + f_{j-1} - 2f_j)$$
$$= -a\delta_x f_c + \tfrac{1}{2}a\Delta x\delta^2_x f$$

$\tfrac{1}{2}|a\Delta x|$ is the numerical diffusivity, say α.

comparison equation $\partial_t f + a\partial_x f = \alpha\, \partial^2_x f$
Dissipation of a sine wave: Let $f = \sin(k(x-at))A(t)$. Without diffusion, this is a convected sine wave. Now:

$$\partial_t \sin(k(x-at))A(t) + a\partial_x \sin(k(x-at))\, A(t) = \alpha\, \partial^2_x \sin(k(x-at))\, A(t) \ \Rightarrow$$

$$d_t A = -\alpha k^2 A \quad \text{so sine wave damps with time} \quad f = \sin(k(x-at))\exp(-\alpha k^2 t).$$

$k=2\pi/\lambda$ so short waves damp rapidly: in one time step decay exponent is

$$\alpha k^2\Delta t = 2\pi^2\, a\Delta t\Delta x/\lambda^2 = 2\pi^2 C\, (\Delta x/\lambda)^2$$

so grid spacing must be small compared to wavelength for accuracy.

2. Automatic upwinding

In CFD *a* could be positive or negative.

1) Could use an `IF` statement:

`IF(a > 0)` $\delta_x f = f_j - f_{j-1} / \Delta x$

`ELSE` $\delta_x f = f_{j+1} - f_j / \Delta x$

2) Without `IF` statement: $a\partial_x f = \tfrac{1}{2}(a+|a|)\, \partial_x f + \tfrac{1}{2}(a-|a|)\, \partial_x f$ called `splitting'

$$a\delta_x f = \tfrac{1}{2}(a+|a|)\, (f_j - f_{j-1})/\Delta x + \tfrac{1}{2}(a-|a|)\, (f_{j+1} - f_j)/\Delta x$$

combining terms shows that this is central + diffusion (1st order upwind)

$$= a/(2\Delta x)(f_{j+1} - f_{j-1}) - \tfrac{1}{2}|a\Delta x|(f_{j+1} + f_{j-1} - 2f_j) / \Delta x^2$$

3. User controlled diffusion: introduce parameter ε in front of $|a|$.

   $\delta f/\delta t = -\,a/(2\Delta x)(f_{j+1} - f_{j-1}) + ½\, \varepsilon\, |a\Delta x|(f_{j+1} + f_{j-1} - 2f_j) / \Delta x^2$

   If $\varepsilon \neq 0$ this is still first order, but ε can be minimized to reduce artificial dissipation. (But, still first order accurate).

   JST scheme has user specified second and fourth order numerical viscosity.

   With Euler explicit

   $f_j^{n+1} = f_j^n - ½\, C(f_{j+1} - f_{j-1})^n + ½\, \varepsilon\, C(f_{j+1} + f_{j-1} - 2f_j)^n$

   The stability criterion is now †

   $1/C \geq \varepsilon \geq C$

   Comparing left to right: $|C|<1$

   Recall diffusion equation: $\alpha\Delta t/\Delta x^2 < 1/2$ for stability.

   $½\, \varepsilon\, |a\Delta x\, \Delta t/\Delta x^2 < 1/2 \rightarrow \varepsilon\, C < 1$ is left constraint.

   Then $\varepsilon \geq C$ says that $\varepsilon_{min} = C$ as the least dissipation consistent with stability.
   (*Laney p.264*) This turns out to be Lax-Wendroff -- next lecture

† Proof:

$f_j^{n+1} = f_j^n - ½\, C(f_{j+1} - f_{j-1})^n + ½\, \varepsilon\, C(f_{j+1} + f_{j-1} - 2f_j)^n \qquad f_j^n \to A^n e^{i\Theta j} \qquad i = \sqrt{-1}$

$G^2 = \|\, 1 - iC \sin\theta + \varepsilon C(\cos\theta - 1)\, \|^2$

This is ≤ 1 if

$C^2 (1-\cos\theta^2) + \varepsilon^2 C^2(\cos\theta - 1)^2 + 2\varepsilon C(\cos\theta - 1) \leq 0$

divide by $\cos\theta - 1$, noting that it is < 0

$-C(1+\cos\theta) + \varepsilon^2 C(\cos\theta - 1) + 2\varepsilon \geq 0$

linear fcn of $\cos\theta$: *if largest when* $\cos\theta = -1 \rightarrow 1 \geq \varepsilon C$ *2Δ wave*

if largest when $\cos\theta = 1 \rightarrow \varepsilon \geq C$ *Long wave must be damped*

C. Numerical methods for simple waves: $\partial_t u + a\,\partial_x u = 0$. Generalize by replacing *au* by flux function *F(u)*. Linear wave is F*(u)=au* . EE is first order; higher order methods RK and LW.

Upwind as (finite vol.) flux interpolation

$$\partial_t u + \partial_x F = \partial_t u + (F_{j+1/2} - F_{j-1/2})/\Delta x$$

with upwind interpolation $= \partial_t u + (F_j - F_{j-1})/\Delta x$

Runge-Kutta revisited (solve N o.d.e.'s for u(j), j=1,N): RK just needs RHS

$\delta_t u_j = -\delta_x F(\mathbf{u}) = \text{RHS}$: Central: $\text{RHS} = -(F(u_{j+1}) - F(u_{j-1}))/2\Delta x$

Upwind: $\text{RHS} = -(F(u_j) - F(u_{j-1}))/\Delta x$

Code: set u(x) to initial value; provide a routine that evaluates RHS; call RK*n*(u,RHS,Δt)

Pseudo-Code; EE and RK are explicit *time-integrators*; RHS is *spatial scheme*

```
    U(:) = F[x(:)]    ! Initial condition
!*********  Integrate in time  **********
    time: DO t = dt,T,dt
             IF(EEx) call EE(N,RHS,t,U,dt)
             IF(RK)  call rk2(N,RHS,t,U,dt)  ! OUTPUT at selected times
   ENDDO time
!*********************************************
    SUBROUTINE RHS(N,t,U,Up)
    F(U)=a*U                  ! For Burger's eqn F = ½U²
      DO j=1,N-1
         jp = j+1   ;  IF(jp == N) jp = 1      ! No need to solve @N
         jm = j-1   ;  IF(jm == 0) jm = N-1    ! N ≡ 1 periodicity
         IF(central)THEN
           Up(j) = -(F(jp)-F(jm))/(2.*dx)    ! central conservation form
         ELSE
           Up(j) = -(F(j )-F(jm))/ dx        ! 1st O upwind cons. form
         ENDIF                               ! Or p*upwind+(1-p)*downwind
      ENDDO
!*********************************************
   SUBROUTINE EE(N,RHS,t,y,dt)
     CALL RHS(N,t,y,yp)
      y(:) = y(:)+yp(:)*dt
   END EE
!*********************************************
   SUBROUTINE rk2(N,RHS,t,y(:),dt)
       CALL RHS(N,t,y,yp)
        y1(:) = y(:)+.5*yp(:)*dt
       CALL RHS(N,t,y1,yp)
        y(:) = y(:)+yp(:)*dt
   END RK
```

D. Lax-Wendroff

Second order in space and time; minimum user specified viscosity ($\varepsilon = C < 1$)

1. Derivation: Taylor series to second order in time
   $u(t+\Delta t) = u(t) + \dot{u}(t)\Delta t + \frac{1}{2}\ddot{u}\Delta t^2 + O(\Delta t^3)$
   For a linear, simple wave $\dot{u}(t) = -a\partial_x\dot{u}$; $\partial_t\dot{u} = -a\partial_x\dot{u} = a^2\partial_x^2 u$
   $u^{n+1} = u^n - a\partial_x u\Delta t + \frac{1}{2} a^2\Delta t^2\partial_x^2 u$
   Looks like numerical diffusion. $\kappa = \frac{1}{2}a^2\Delta t$; $2\kappa\Delta t/\Delta x^2 = (a\Delta t/\Delta x)^2 = C^2 < 1$ for stability.
   (Recall upwind $\kappa = \frac{1}{2}\varepsilon\, a\Delta x$ so $\varepsilon \rightarrow a\Delta t/\Delta x = C$)
   Use central differencing.
   $u^{n+1} = u^n - C(u_{j+1} - u_{j-1}) + \frac{1}{2} C^2 (u_{j+1} - 2u_j + u_{j-1})$

2. Looks like (*1st order*) upwinding with $\varepsilon = C$ in `user defined' artificial viscosity; nevertheless, is 2nd order in space and time.

   Recall stability $C \leq 1$ and $1/C \geq \varepsilon \geq C$; so $\varepsilon = C$ is minimum viscosity consistent with stability: Hence, L-W has min dissipation

3. Pseudo-code for $u_j^{n+1} = u_j^n - C(u^n_{j+1} - u^n_{j-1}) + \frac{1}{2} C^2((u^n_{j+1} - 2u^n_j + u^n_{j-1})$

```
initialize U(:)
DO t=dt,T
   Un(:) = U(:)    ! Don't overwrite     1,2...J,J+1,J+2,..
  DO j=1,J-1       ! identify J <-> 1    1,2,..J, 1,  2 ,..
     jp = j+1 ; if(jp == J+1) jp= 2
     jm = j-1 ; if(jm == 0) jm=J-1
     U(j)= Un(j)-½C(Un(jp)-Un(jm))+½C²(Un(jp)-2Un(j)+Un(jm))
   ENDDO
  u(J)=u(1)
  !** output u(x,t)
  ENDDO
```

(or, less memory:

```
   DO t=dt,T
      ss = u(J-1)   !  periodicity J ≡ 1
    DO j=1,J-1
       jp  = j+1  ; IF(jp == J) jp=1
       s   = u(j)  !save
       u(j) = u(j) -½C(u(j+1)-ss)+ ½C² (u(jp)-2u(j)+ss)
       ss = s  ! j-1 value
    ENDDO
  ENDDO)
```

4. Comments:
   a. Generalize to flux function:

$$\partial_t u = -\partial_x F(u) \;\; ; \;\; \partial^2_t u = -\partial_x [\partial_u F \, \partial_t u] = \partial_x [\partial_u F \, \partial_x F(u)]$$

   Let $a(u) \equiv \partial_u F(u)$. For Burger's equation $F= ½ u^2$, a=u; linear wave eqn F=au

$$u^{n+1}= u^{n} - \Delta t \delta_x F(u) + ½ \Delta t^2 \delta_x [a(u) \, \delta_x F(u)]$$

   Apply central differencing (treat a(u) correctly).

   b. L-W for Burger's equation (a=u)

$$u_j^{n+1} = u_j^n - \Delta t \, ½(F_{j+1} - F_{j-1})^n / \Delta x + ½ \Delta t^2 \, ½ \, [a_{j+1/2} (F_{j+1} - F_j) - a_{j-1/2} (F_j - F_{j-1})]^n / \Delta x^2$$

   CFL: $|a_{max}| \Delta t/\Delta x \le 1$

   c. Two-step Lax-Wendroff (leads to MacCormick)

$$u^{n+1}= u^n + \dot{f}(t)\Delta t + ½ \ddot{u} \Delta t^2 = u^n + \Delta t \, \partial_t (u + ½ \, \partial_t u \, \Delta t)$$

   Step 1: $u^* = u^n - ½ a \, \Delta t \, \partial_x u^n$; Step 2: $u^{n+1}= u^n - \Delta t a \partial_x (u^*)$

   Second step is $u_j^{n+1}= = u_j^n - C(u^*_{j+1/2} - u^*_{j-1/2})$

   $C = a\Delta t/\Delta x$

   Step 1: For all j

$$u^*_{j+1/2} = u^n_{j+1/2} - ½ \, a \partial_x u \, \Delta t = ½ \, (u_{j+1} + u_j) - ½ \, C(u^n_{j+1} - u^n_j)$$

   [NB: $u^*_{j-1/2} = u^n_{j-1/2} - ½ \, C(u^n_j - u^n_{j-1})$]

   Step 2: for all j

$$u_j^{n+1}= u_j^n - C(u^*_{j+1/2} - u^*_{j-1/2})$$

   For the student to verify that L-W scheme is recovered

E. MacCormick's method

Like RK2, properties are analogous to LW; does not require second derivative w.r.t. x

1. Take half step using downwind, then half step using upwind, or *vice-versa*

2. Consider equation $\partial_t u = -\partial_x F(u)$ and assume $\partial_u F(u) > 0$ (right moving wave)

   step 1

   $u_j^* = u_j^n - \Delta t/\Delta x \, (F_{j+1} - F_j)$ *downwind*

   step 2 (c.f., midpoint rule)

   $u_j^{n+1} = ½(u_j^n + u_j^*) - ½ \, \Delta t/\Delta x \, [F(u_j^*) - F(u_{j-1}^*)]$ *upwind*

   NOTE:

   $½(u_j^n + u_j^*) = u_j^n - ½ \, \Delta t/\Delta x \, (F_{j+1} - F_j)$ is 1/2 step with downwind I

3. For example, Linear flux function F = au ; C= aΔt/Δx

```
DO j (=2,J-1, or periodic)
    us(j) = u(j) -C(u(j+1)-u(j))
ENDDO
DO j
    u(j) = (us(j)+u(j))/2 - ½C (us(j) - us(j-1))
ENDDO
```

4. Check (or leave for students?)

$$u_j^{n+1} = \tfrac{1}{2}((u_j^*=)\ u_j^n - C(u_{j+1}^n - u_j^n) + u_j^n) - \tfrac{1}{2}C\ (\ (u_j^* - u_{j-1} =)\ u_j^n - u_{j-1}^n - C[u_{j+1}^n - u_j^n - (u_j^n - u_{j-1}^n)]$$

$$= u_j^n - \tfrac{1}{2}C\ (u_{j+1}^n - u_{j-1}^n)) + \tfrac{1}{2}C^2\ (u_{j+1}^n - 2u_j^n + u_{j-1}^n)$$

∴ Same as Lax-Wendroff

C< 1 for stability or aΔt < Δx